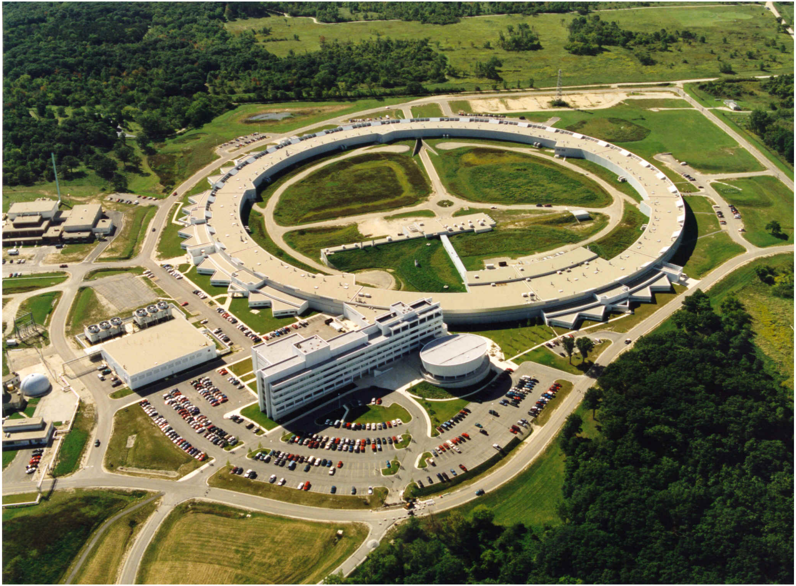
Designing Particle Accelerators Using Derivative-free Optimization

Jeffrey Larson

Argonne National Laboratory

February 6, 2015

Motivation



APS: $467M to build; tens of millions to operate.

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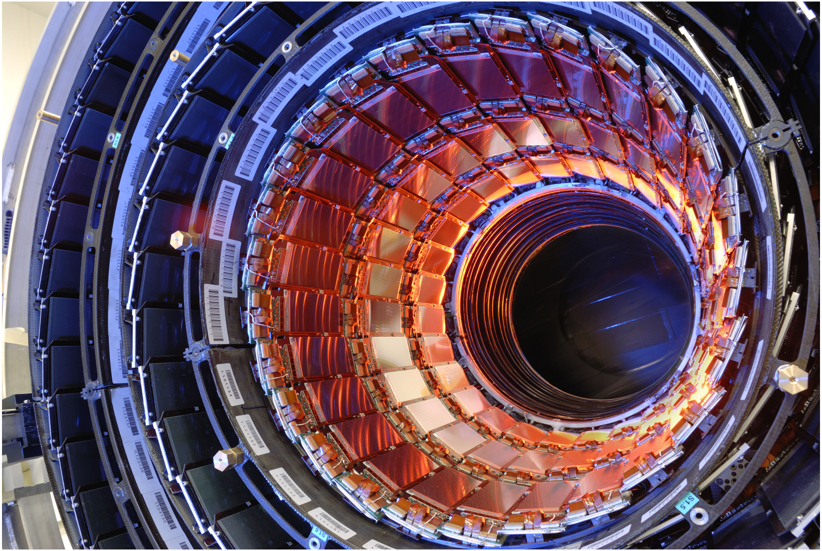

LHC: \$4.75B to build; \$1B to operate; \$0.25B computation

Motivation

Mira: $180M to build; $4M to operate; 3.9 Megawatts

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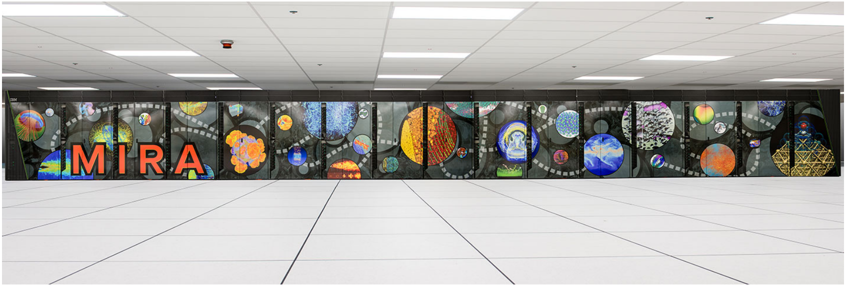

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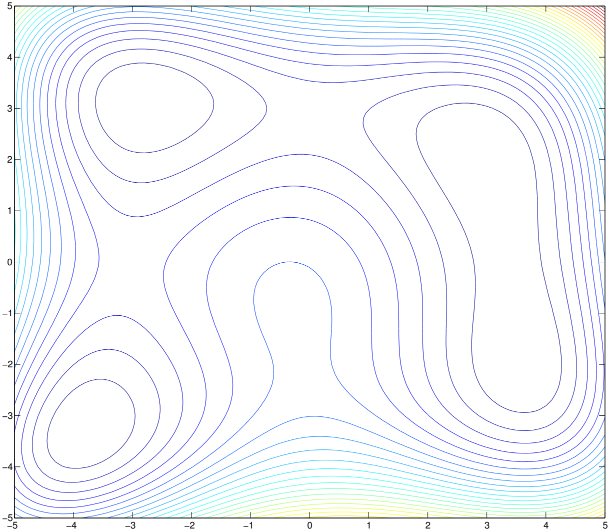

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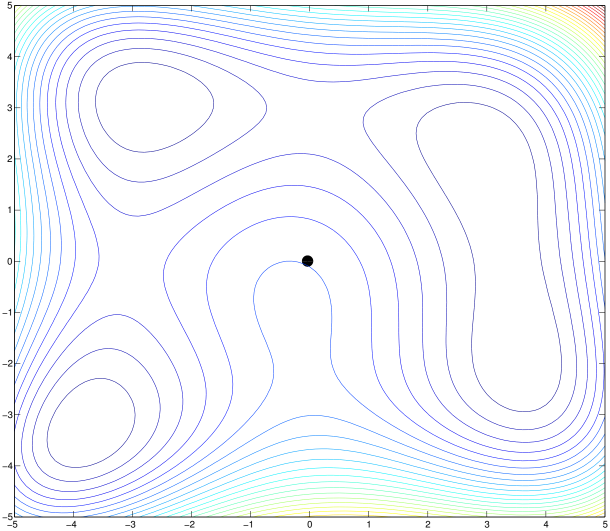

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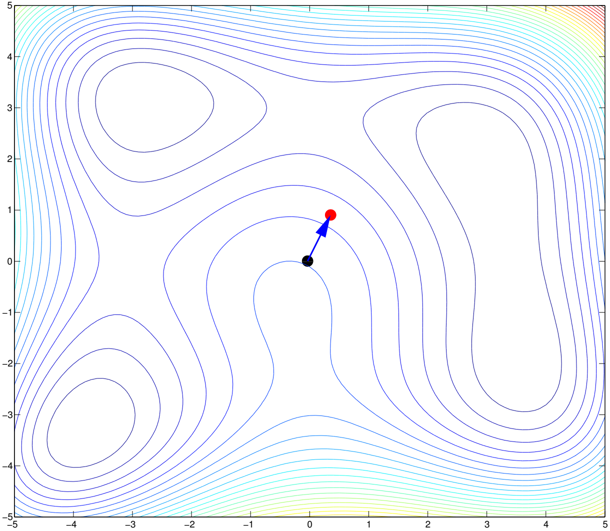

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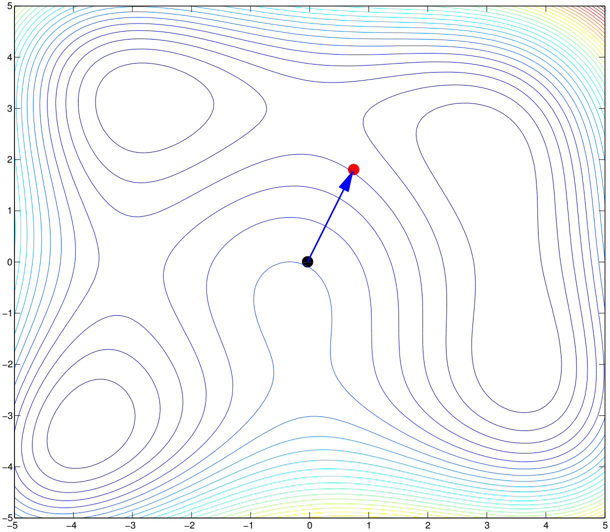

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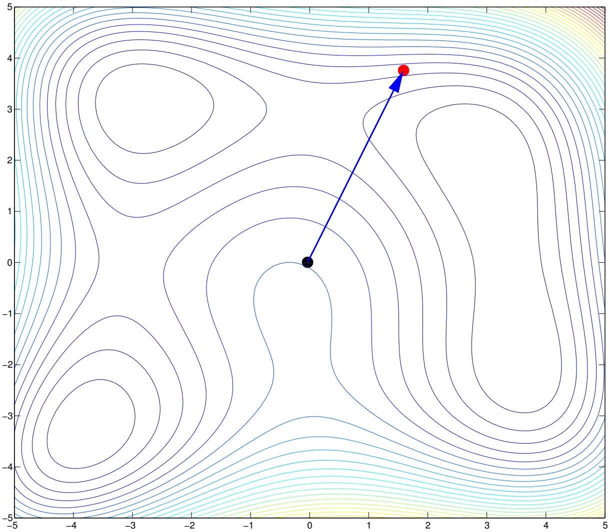

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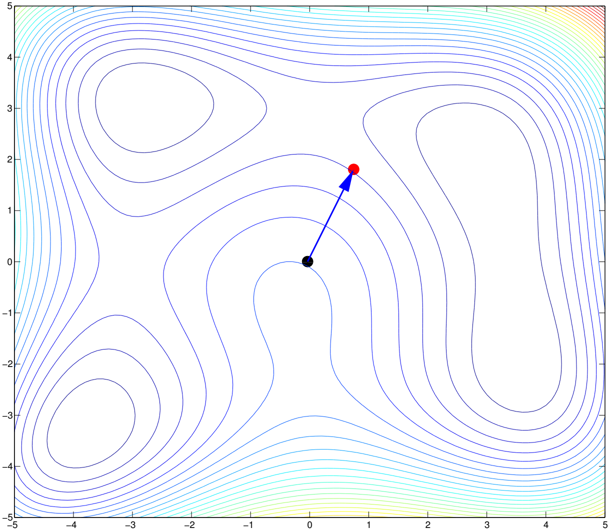

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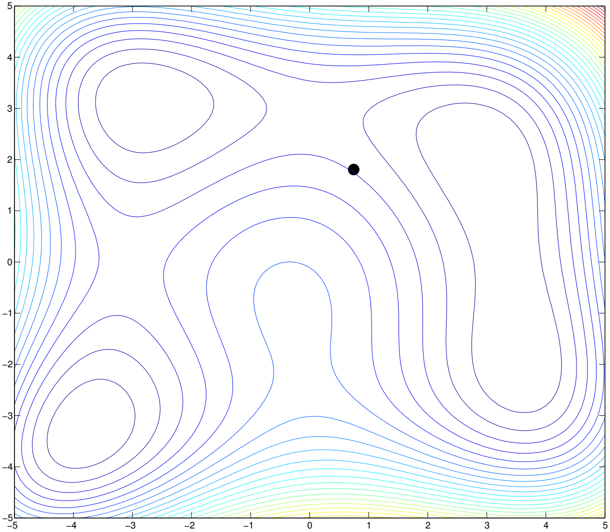

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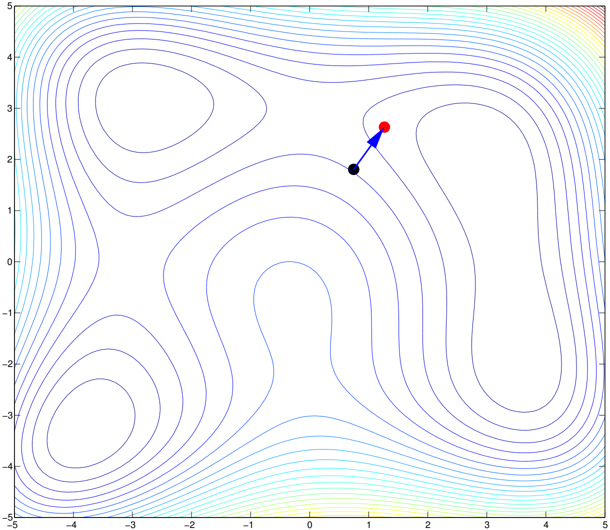

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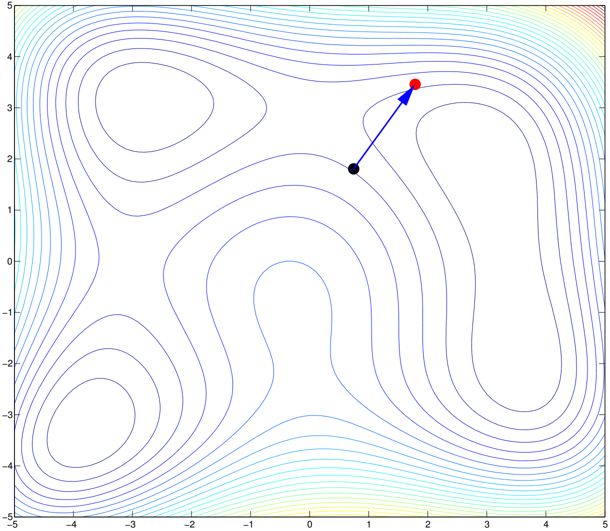

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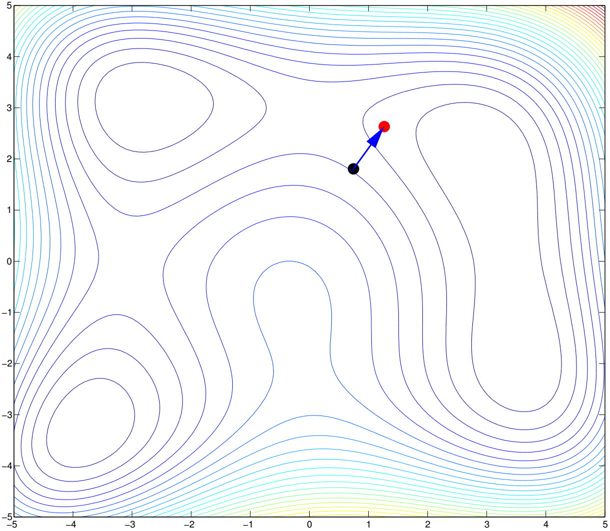

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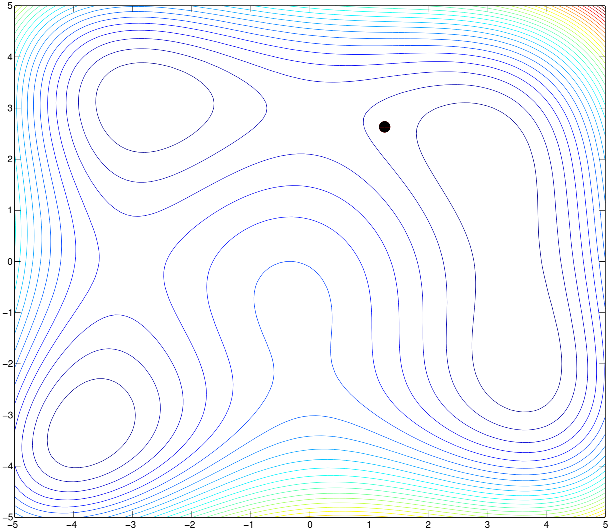

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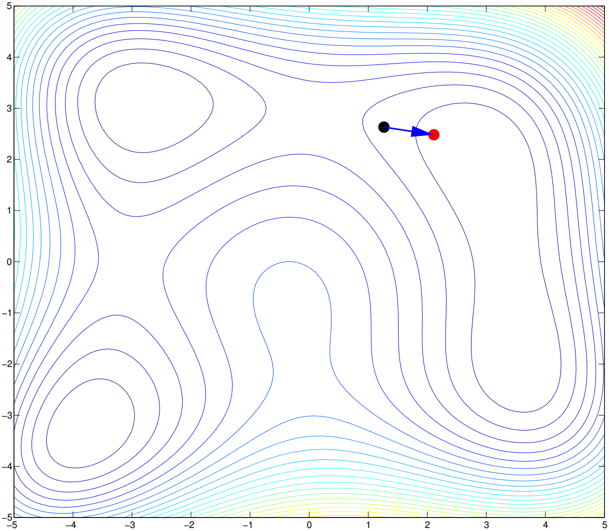

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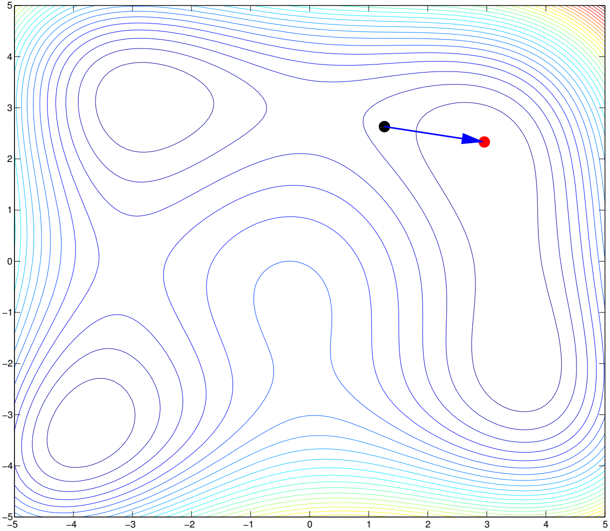

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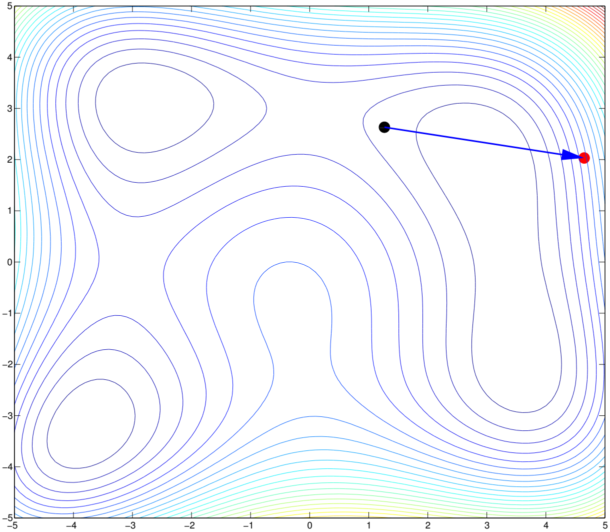

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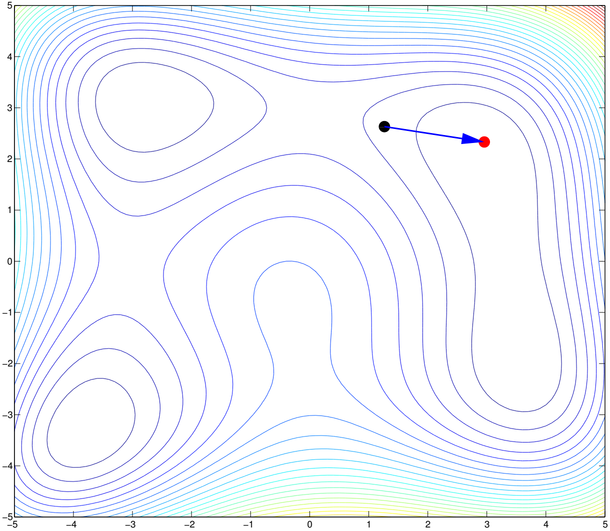

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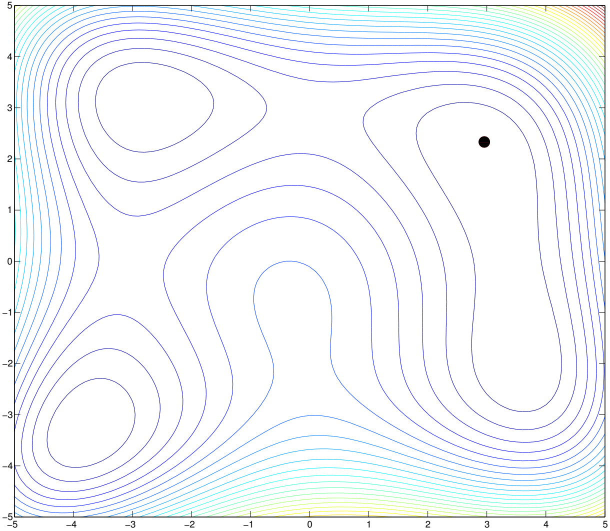

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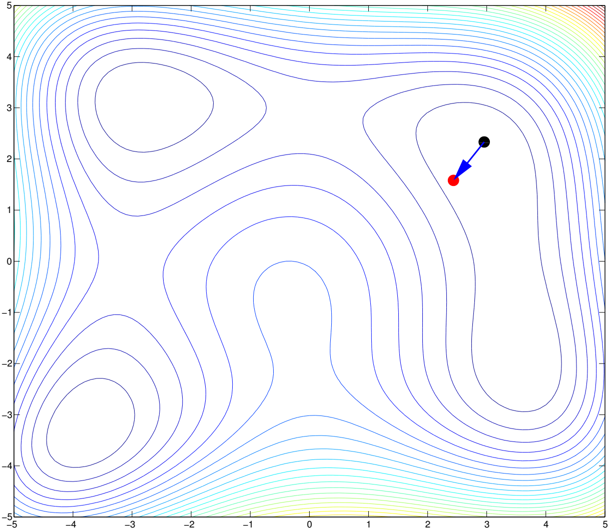

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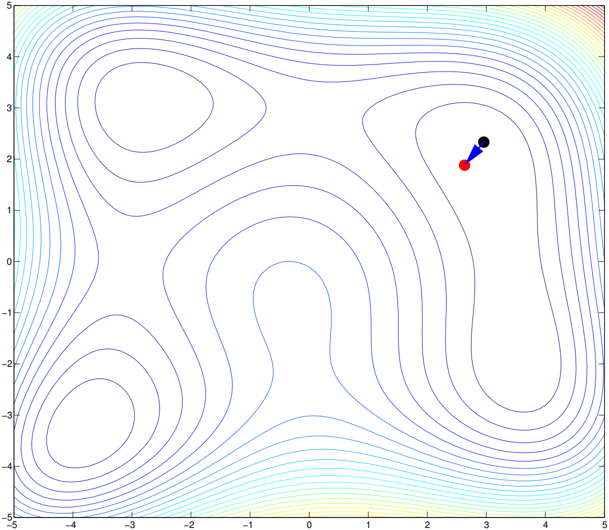

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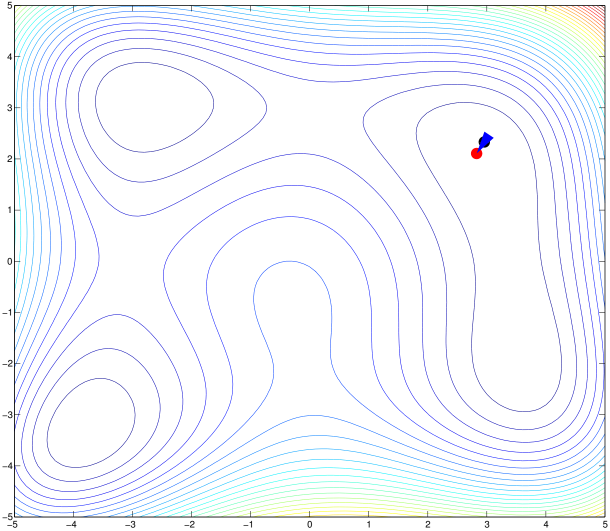
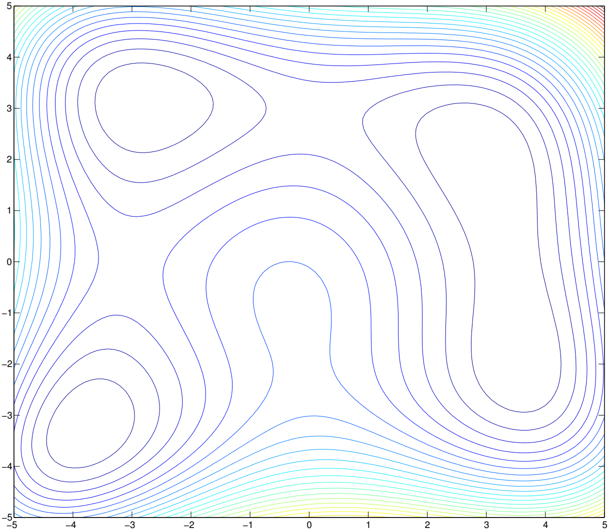


Trust Region Example



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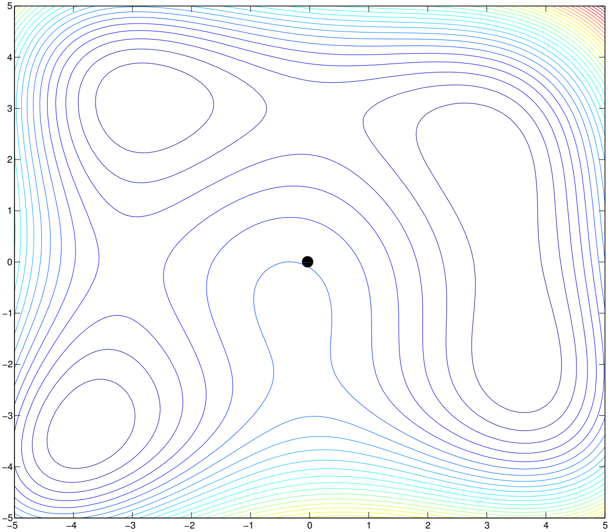

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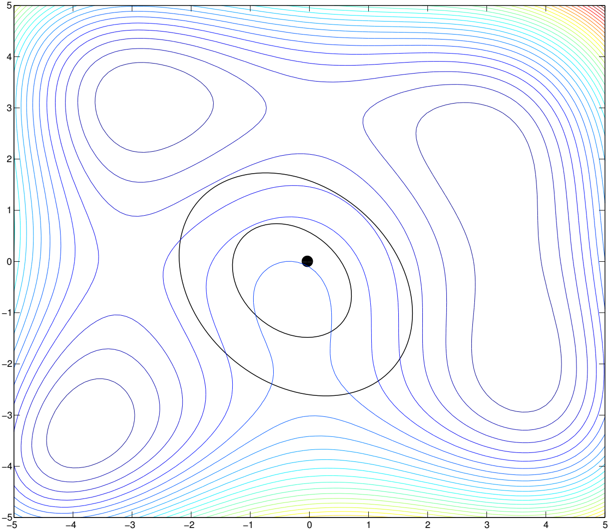

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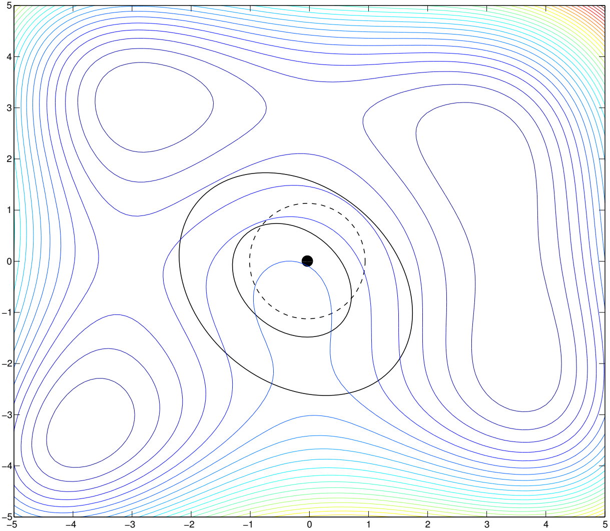

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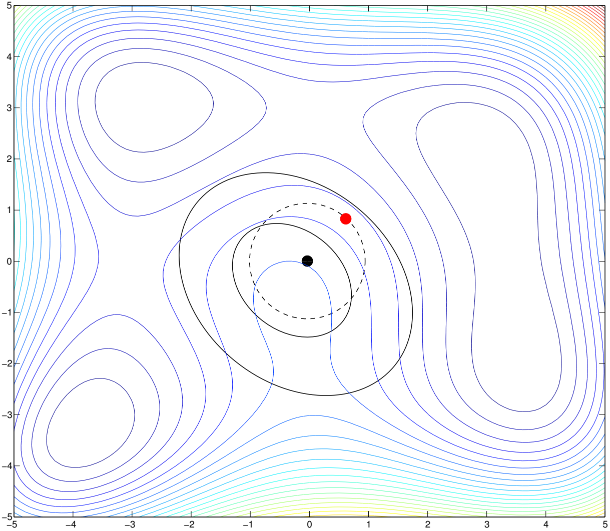

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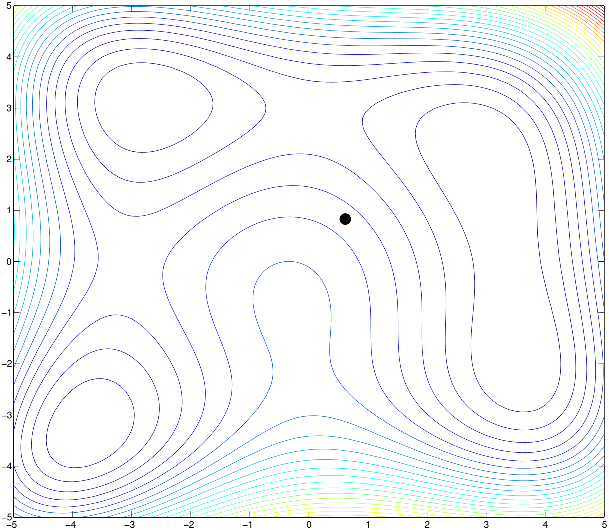

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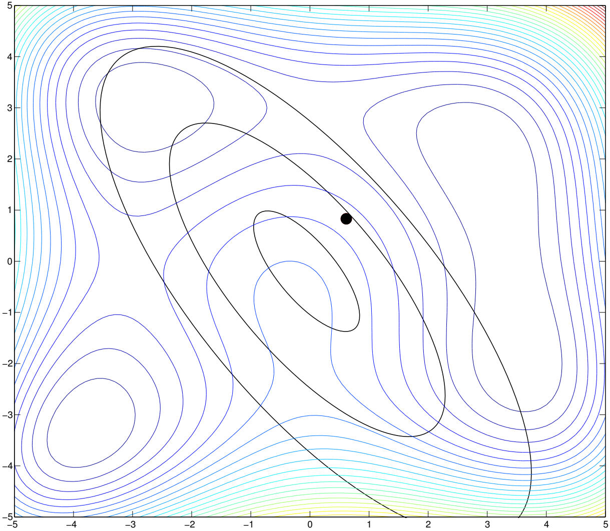

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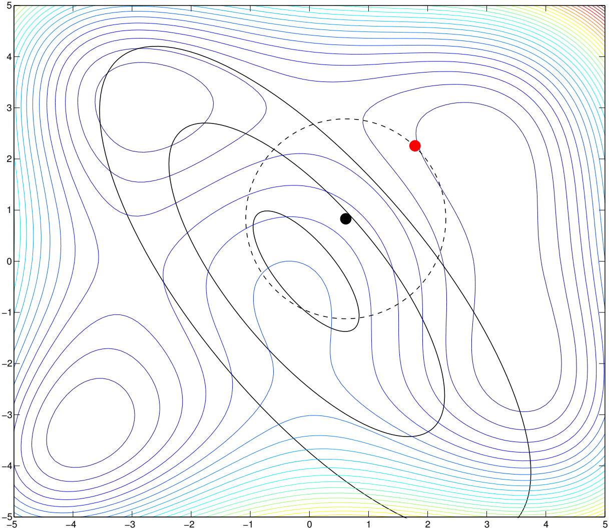

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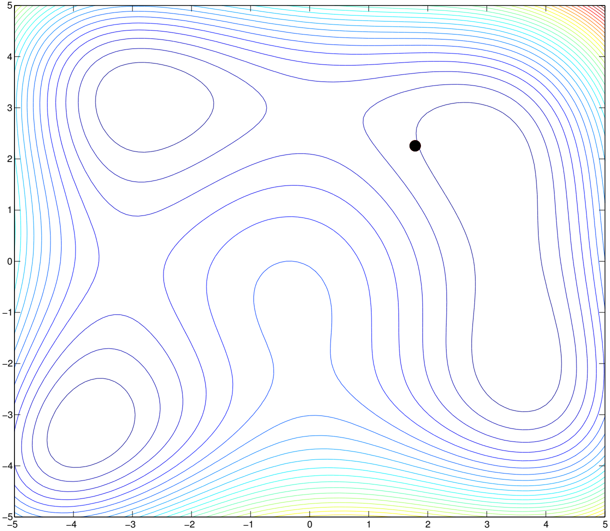

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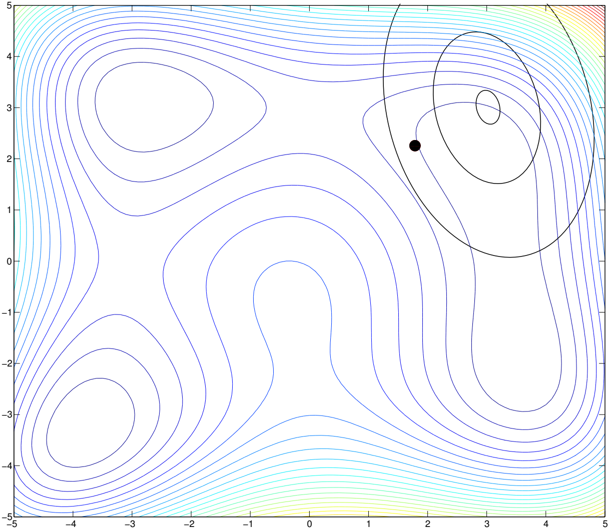

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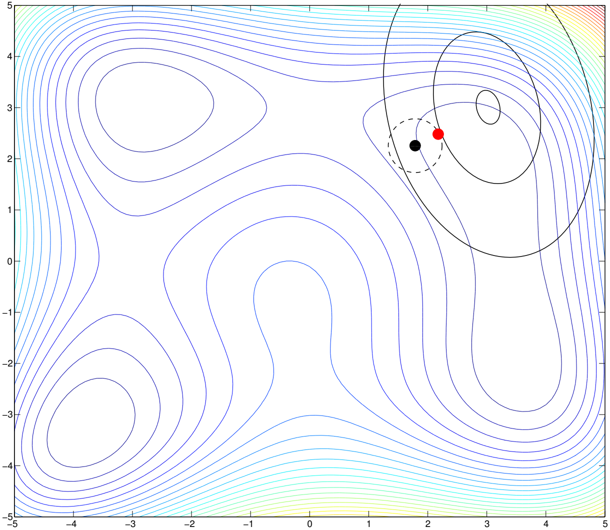

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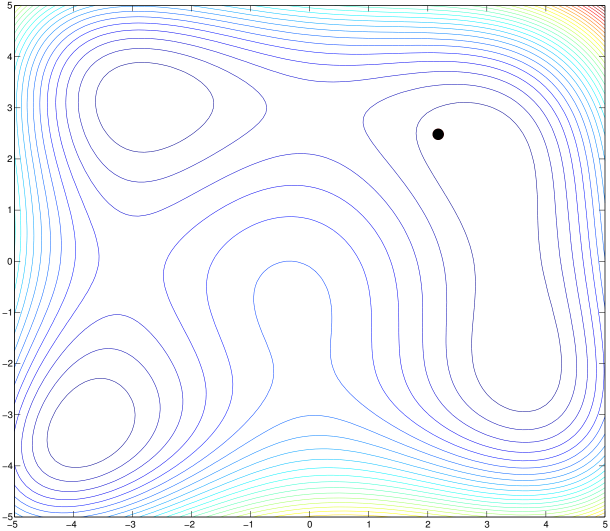

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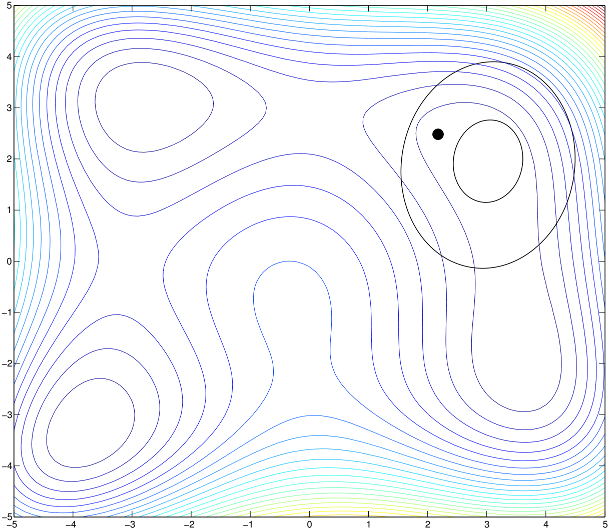

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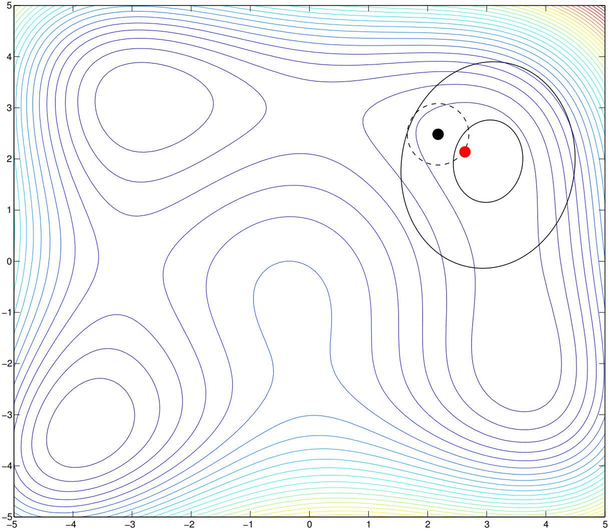

Optimizing simulations

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x)$$

$$\textbf{subject to: } x \in \mathcal{D} = \{x : -\infty < l \leq x \leq u < \infty\}$$

$$\nabla f(x) \text{ is not available}$$

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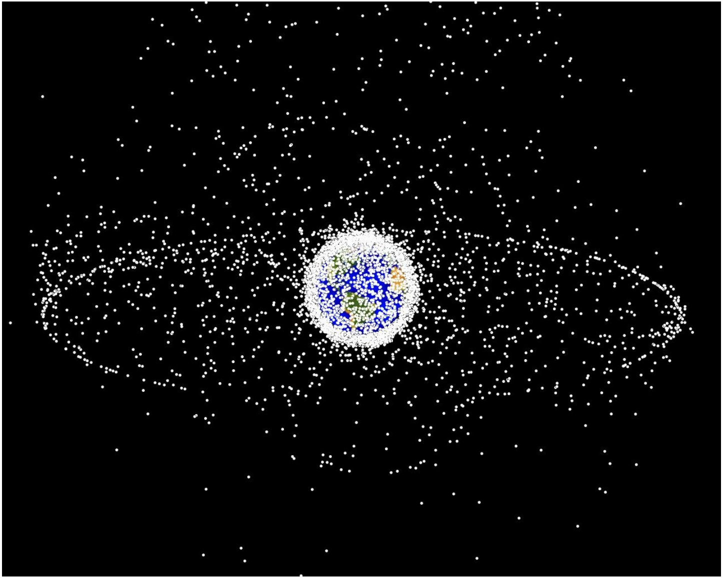
- Disclaimer: If the problem has derivatives please use them!

Optimizing simulations

Derivative-free optimization problems show up throughout the world

- Engine design
- Physical experiments
- Tribology
- Satellite planning

Satellite Collision Avoidance



Courtesy NASA/JPL-Caltech

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  - Use the least amount of fuel as possible
- What would you do?

Try it yourself

MATLAB

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Process should hopefully be described to a computer.

Common first thoughts

- Random Guessing
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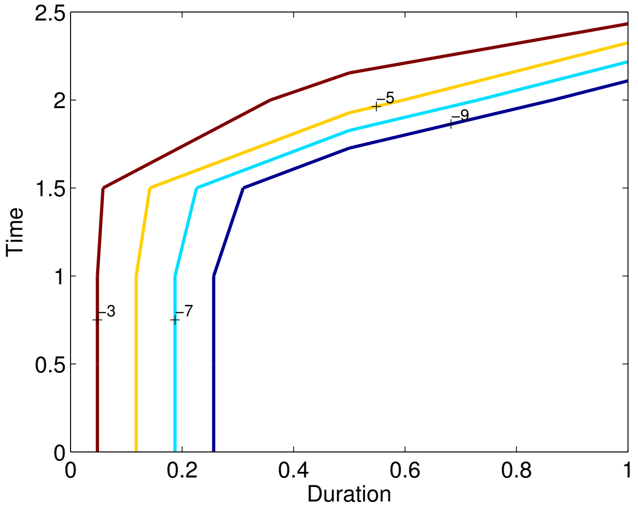
- Random Guessing
  - Not very elegant
  - Evaluate points close to previous points
  - Needs some sort of finishing step
- Finite-differences can be problematic
  - $n + 1$ or $2n + 1$ evaluations at every point
  - Simulations are often noisy

Grid Search



[0:0.5:1] by [0:0.5:2.5] $\approx$ 6 minutes

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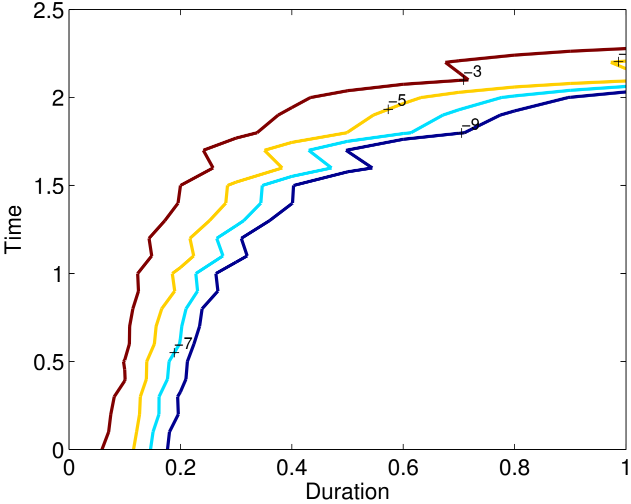

[0:0.1:1] by [0:0.1:2.5] $\approx$ 1.5 hours

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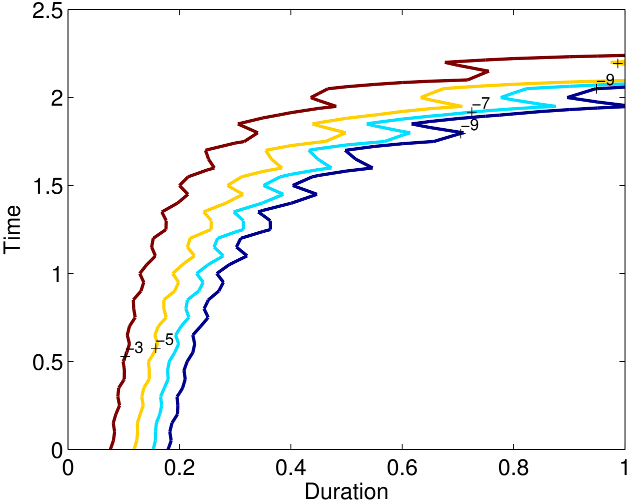

[0:0.05:1] by [0:0.05:2.5] $\approx$ 6 hours

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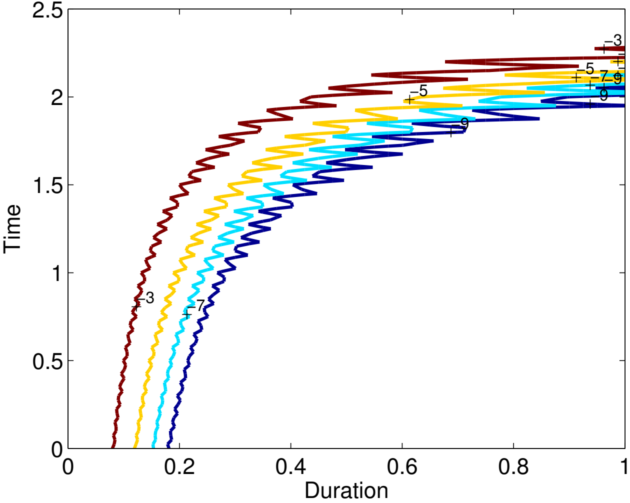
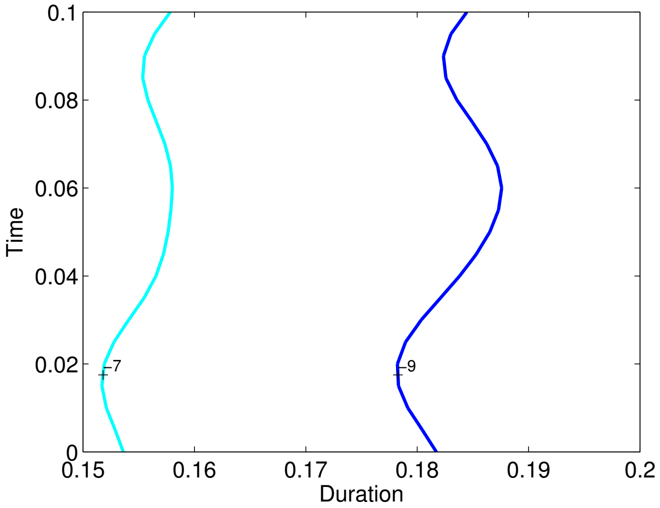


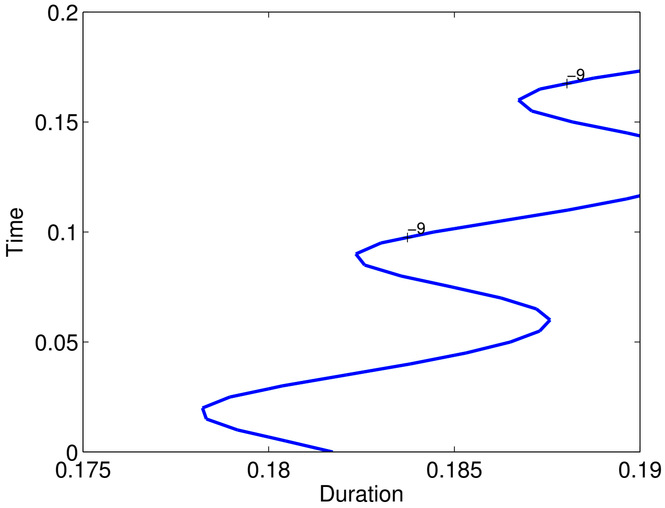
[0:0.025:1] by [0:0.025:2.5] $\approx$ 1 day

Grid Search



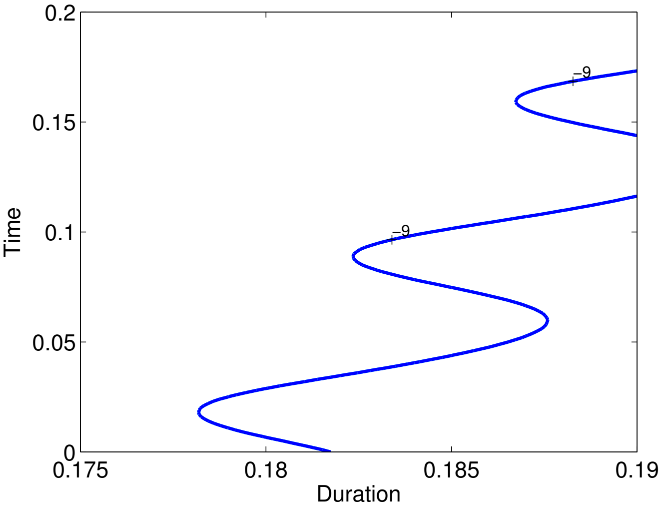
[0.15:0.005:0.2] by [0:0.005:0.1] $\approx$ 1.3 hours

Grid Search



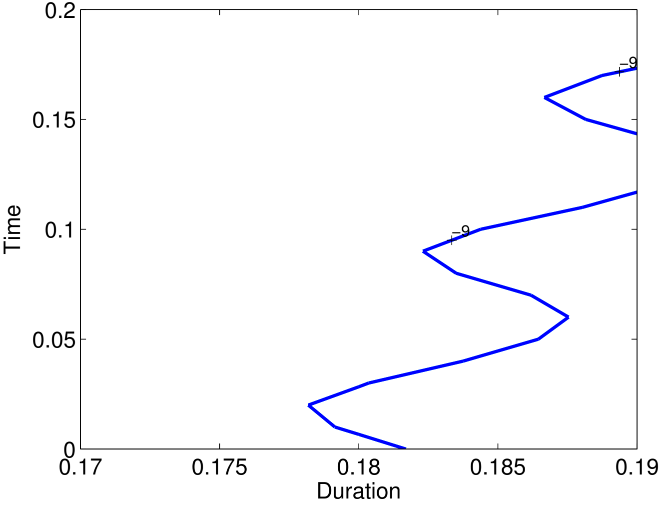
[0.175:0.005:0.19] by [0:0.005:0.2] $\approx$ 55 minutes

Grid Search



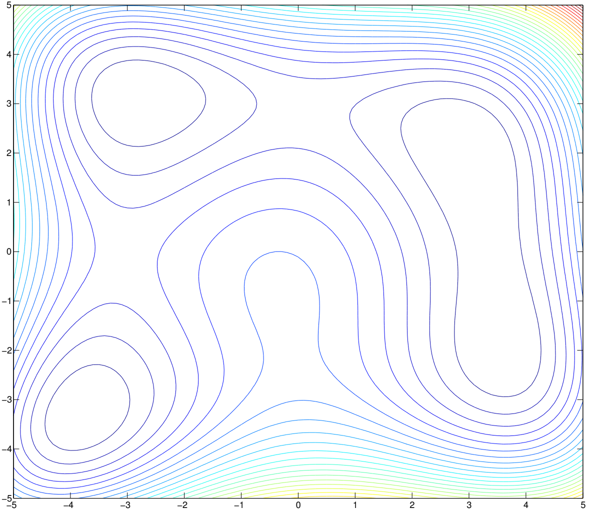
[0.175:0.001:0.19] by [0:0.001:0.2] $\approx$ 18 hours

Grid Search



[0.17:0.01:0.19] by [0:0.01:0.2] $\approx$ 20 minutes

Coordinate Search



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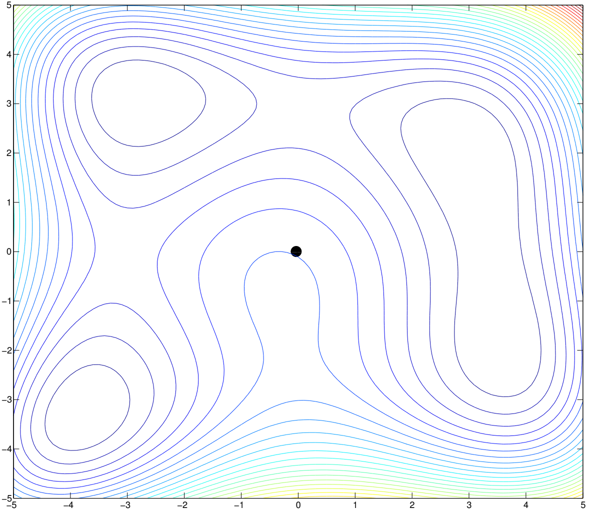

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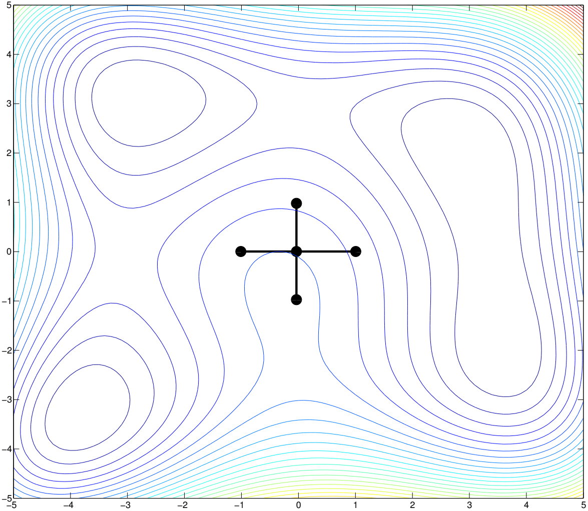

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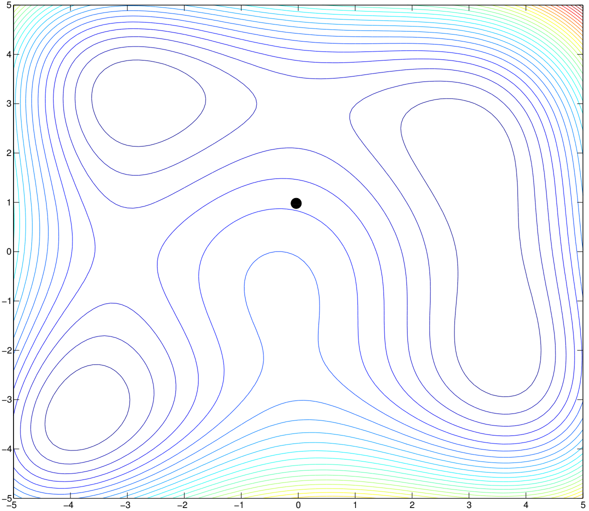

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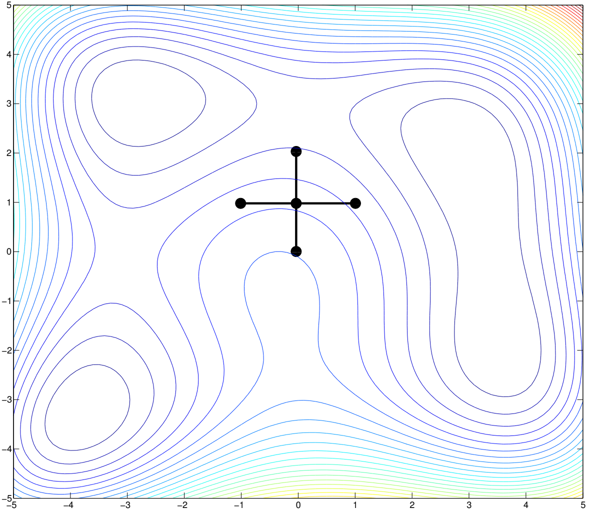

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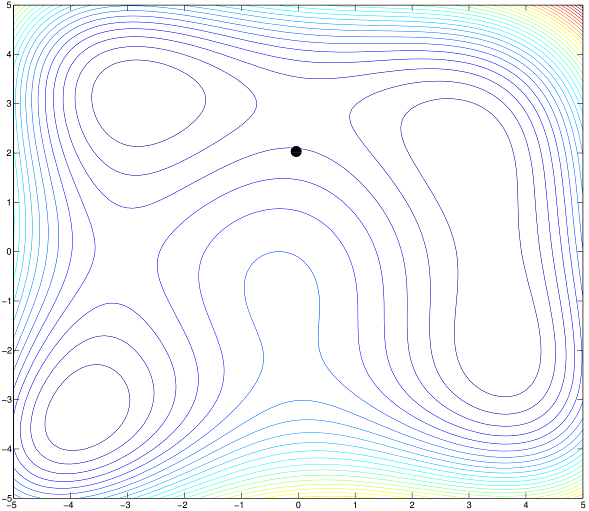

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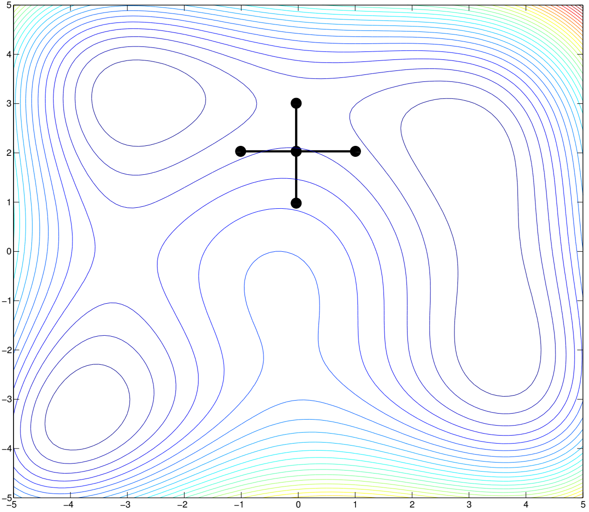

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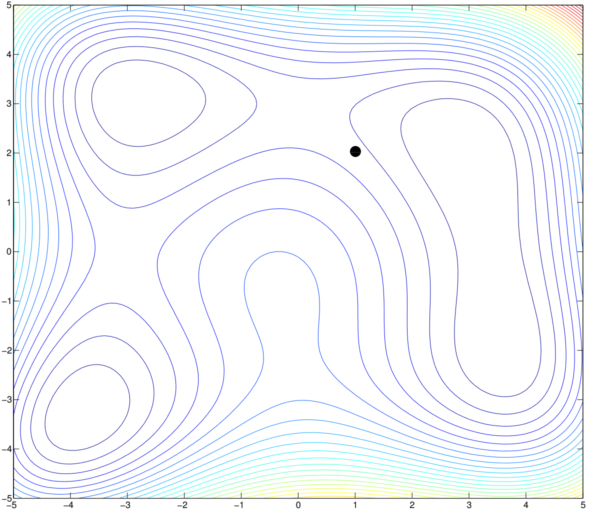

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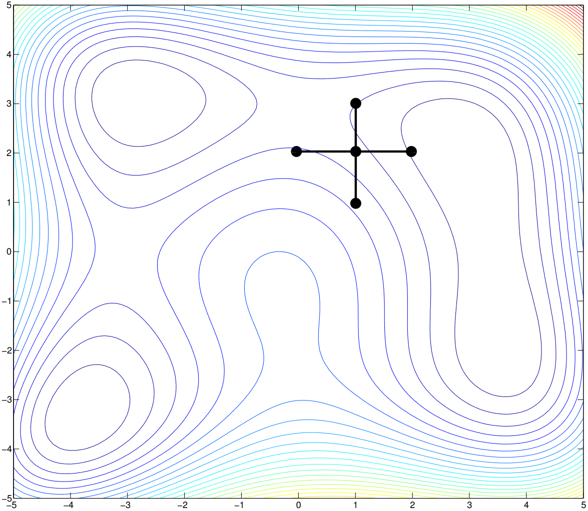

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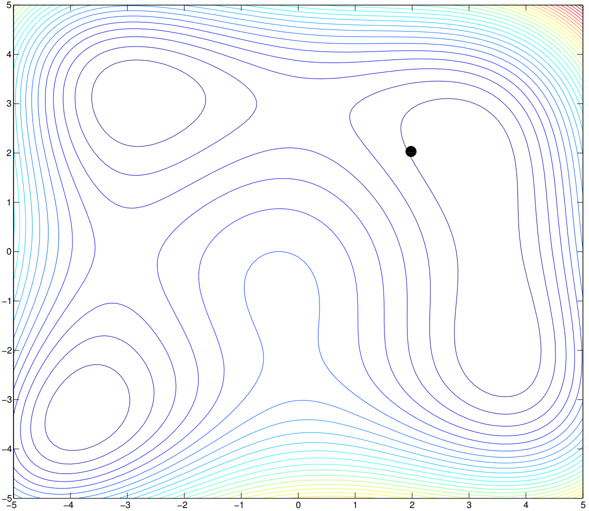

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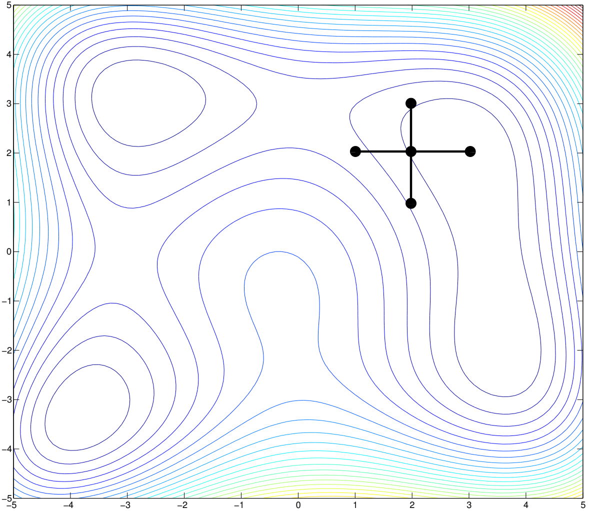

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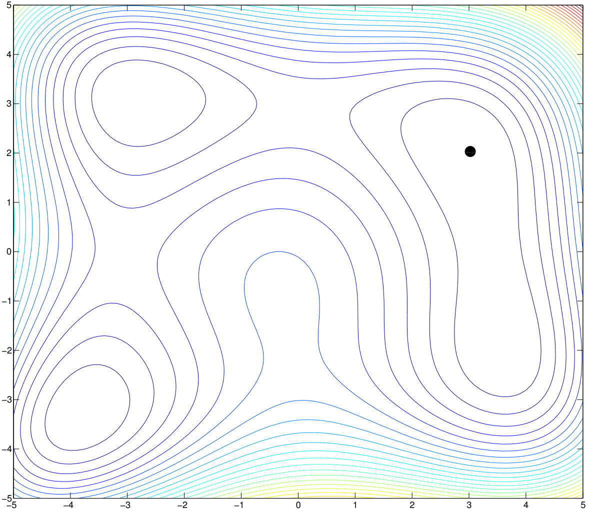

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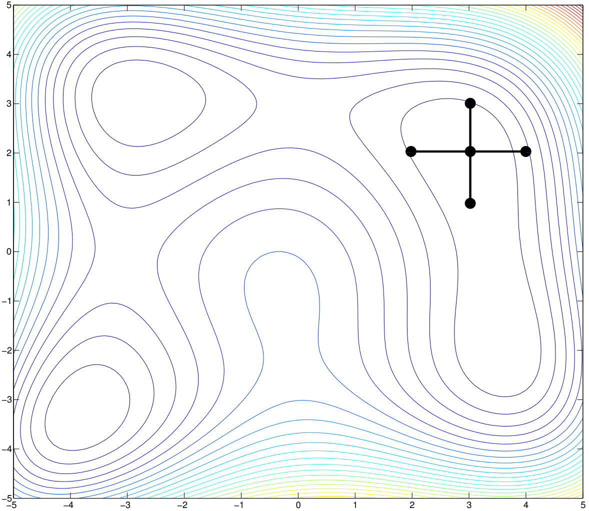

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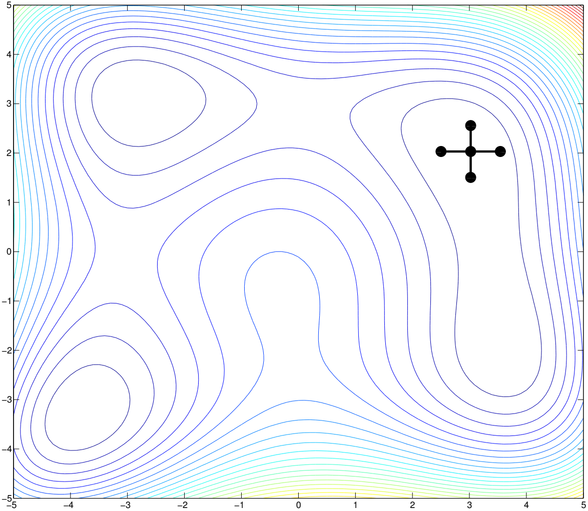

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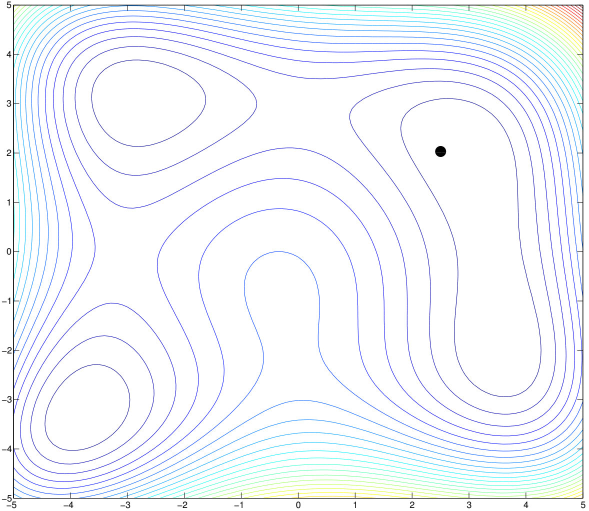

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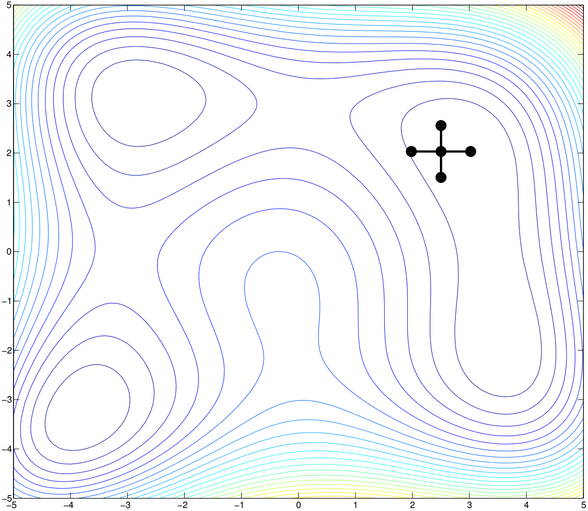

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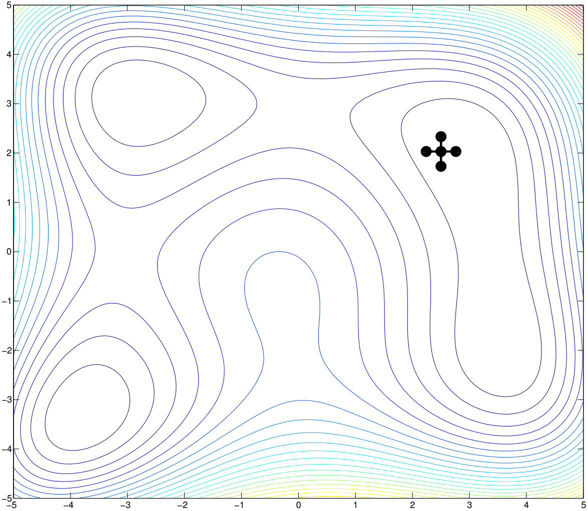
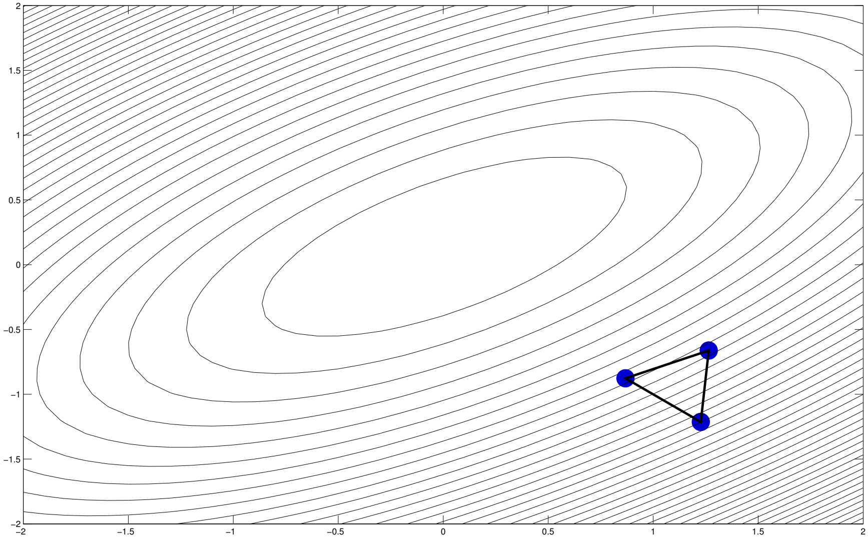


Nelder-Mead



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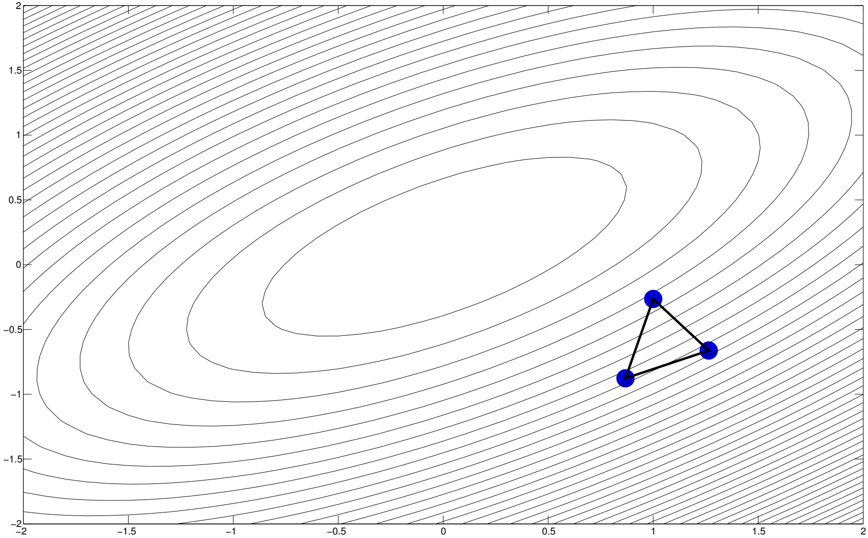

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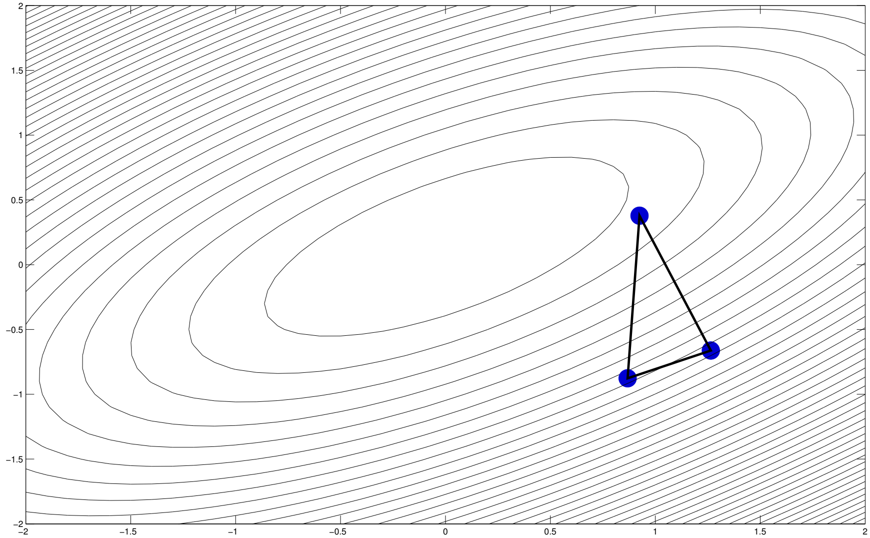

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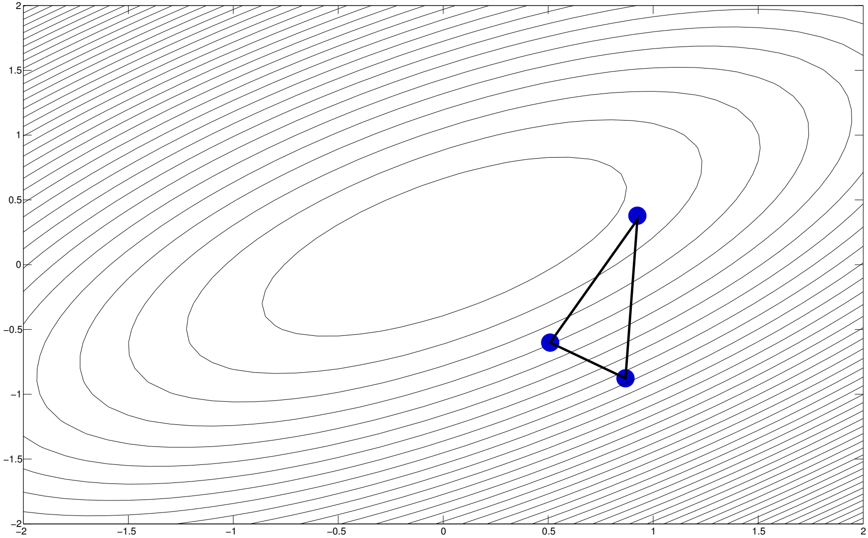

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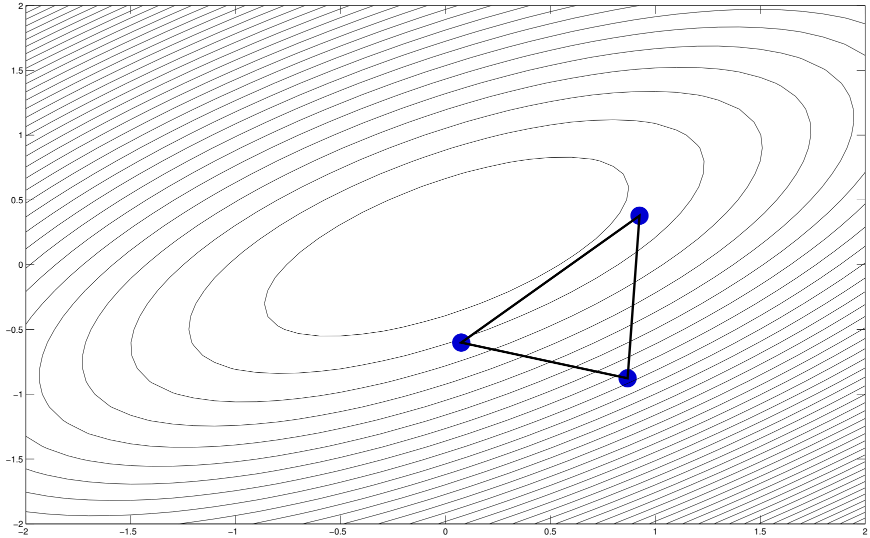

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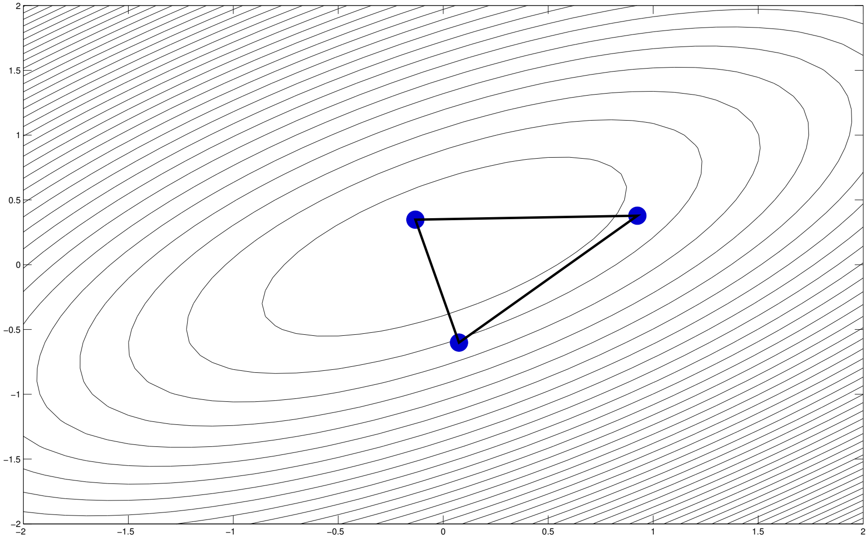

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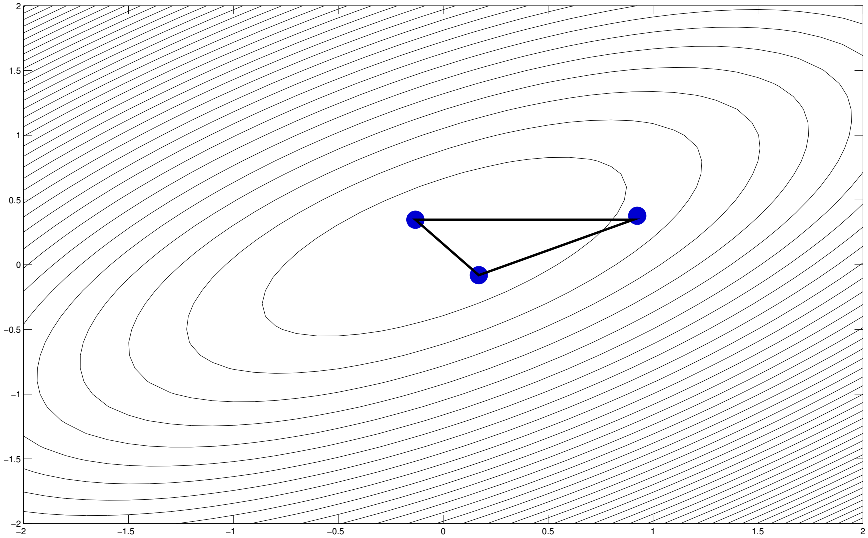

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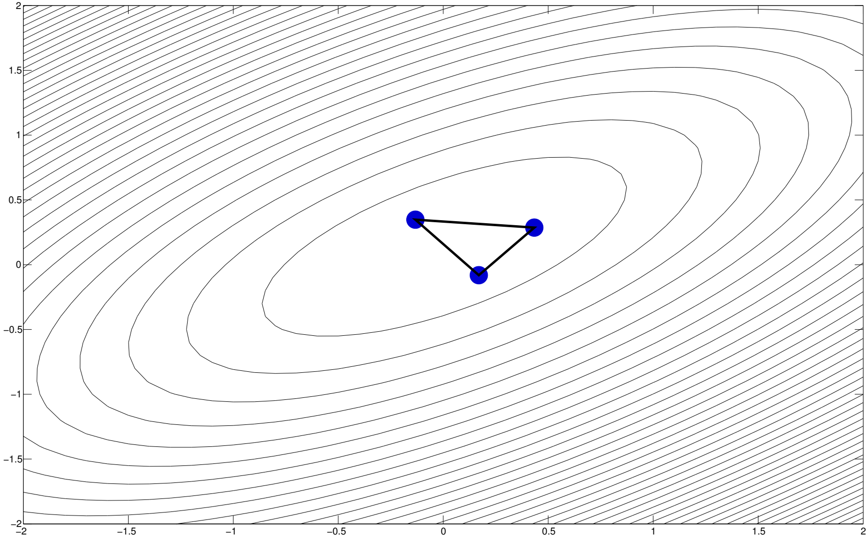

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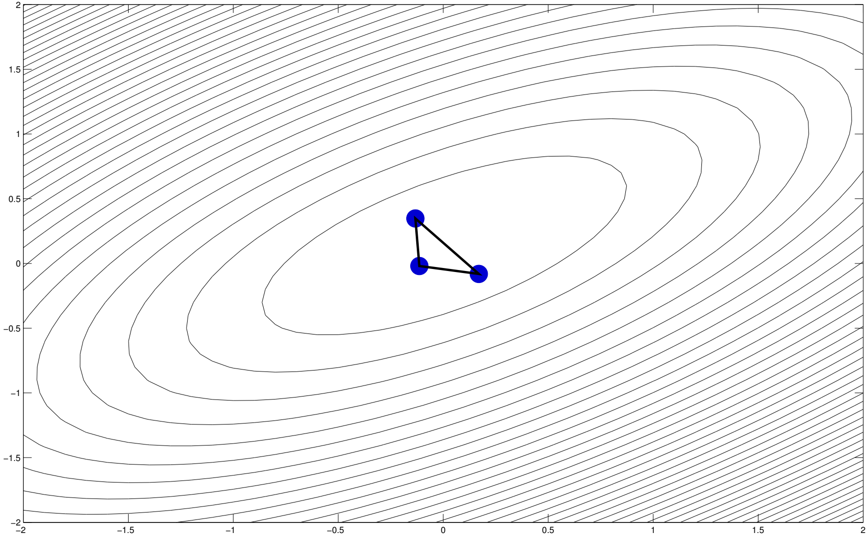

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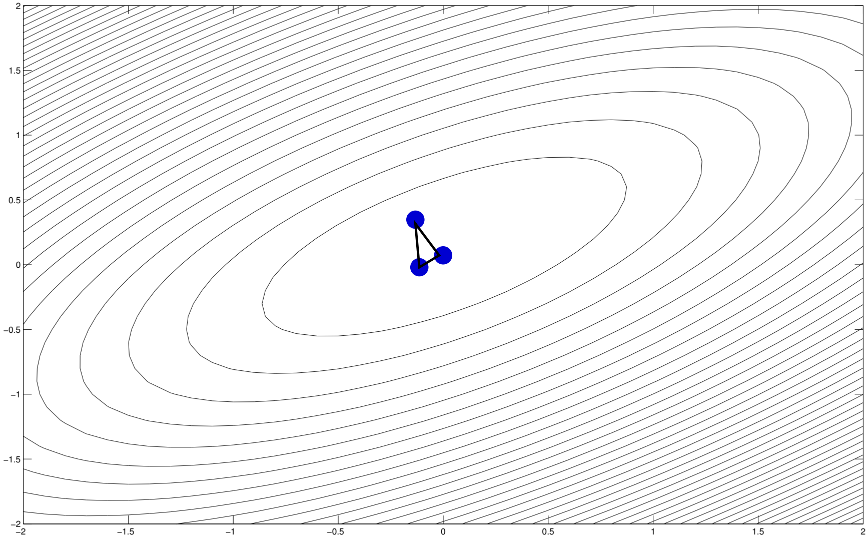
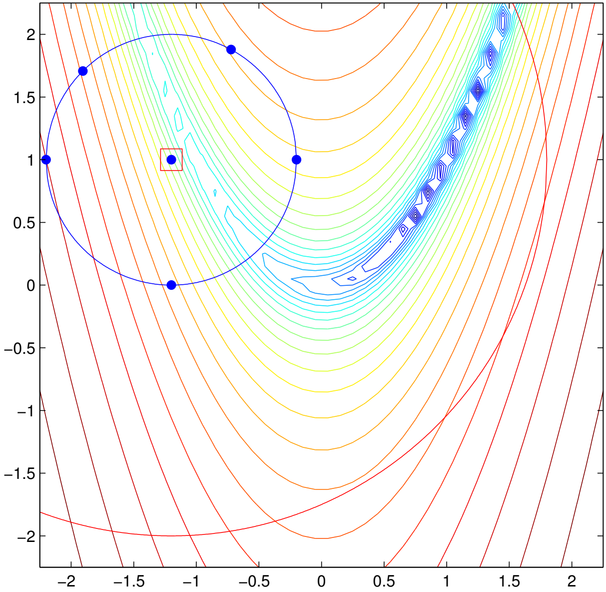


Model-based methods - Interpolation



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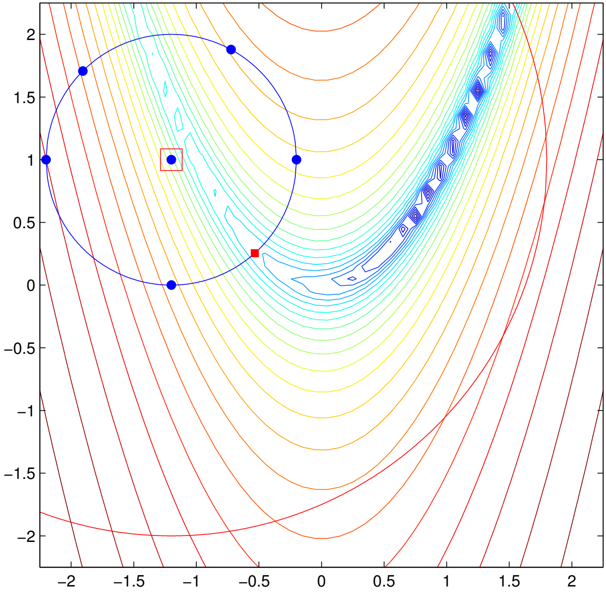

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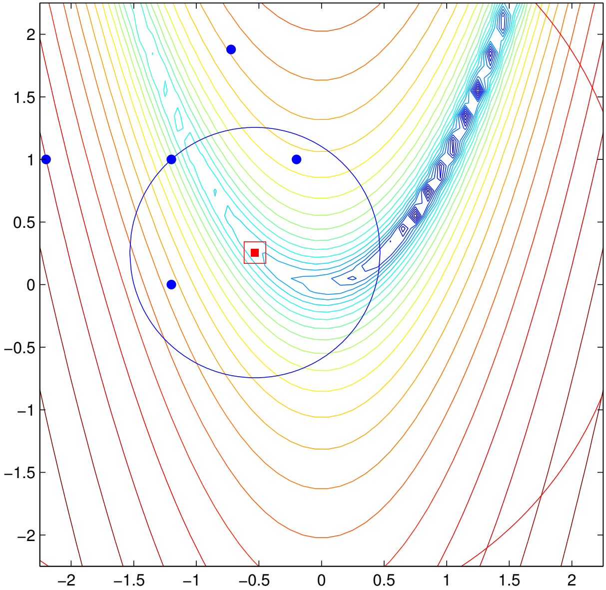

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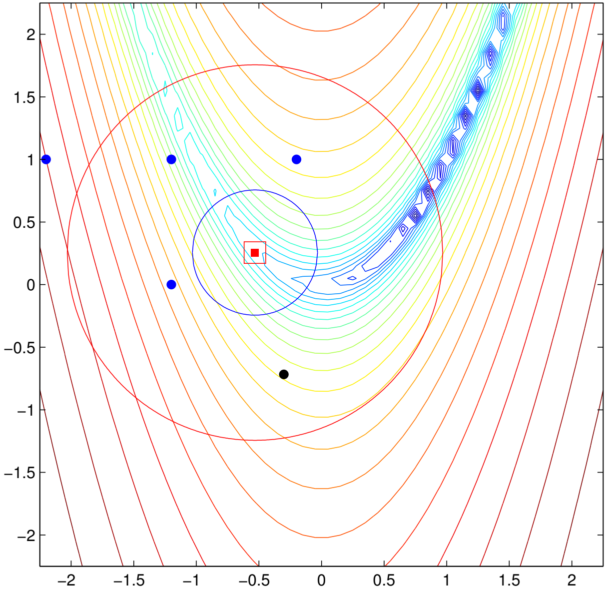

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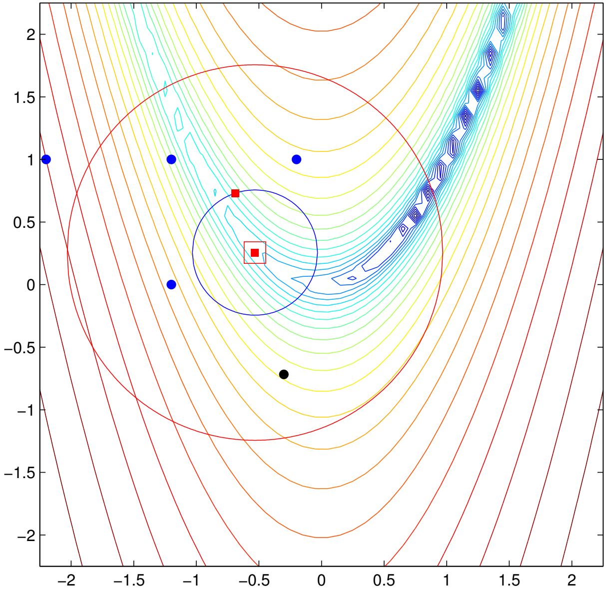

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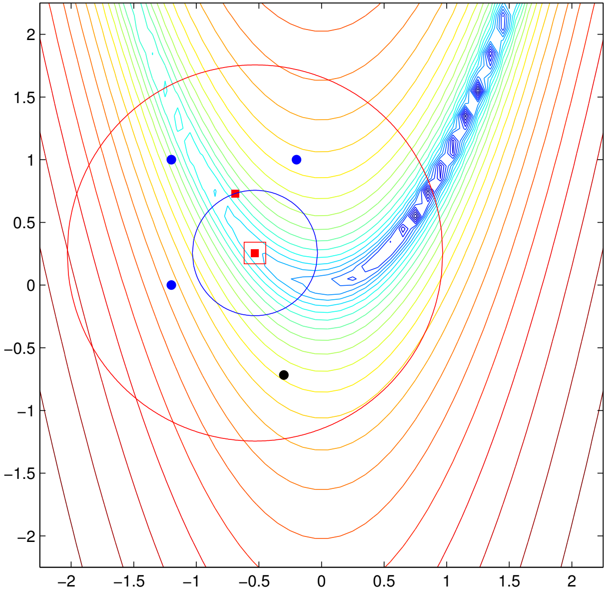

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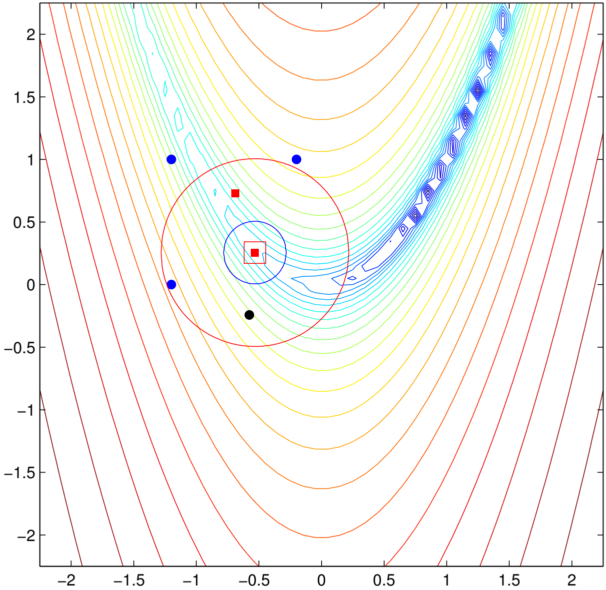

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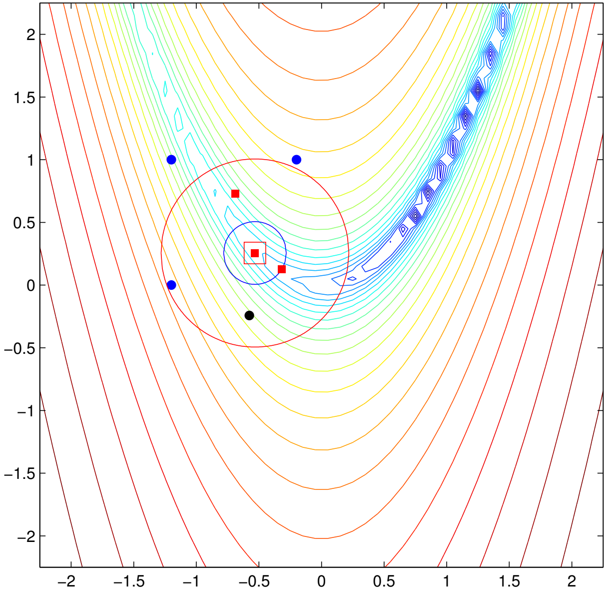

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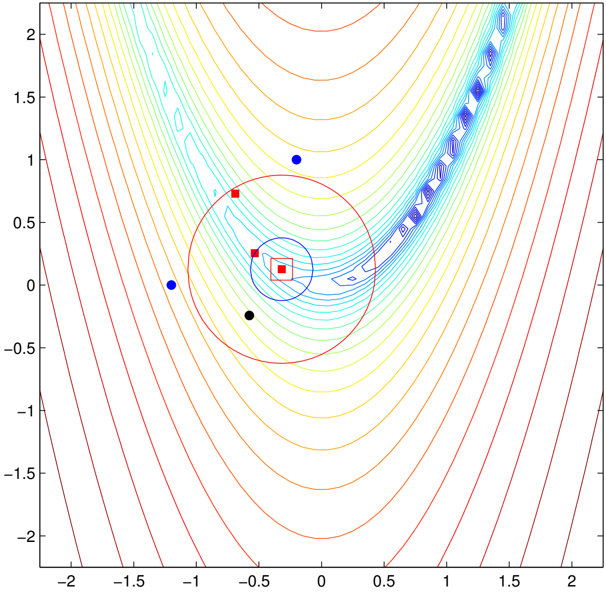

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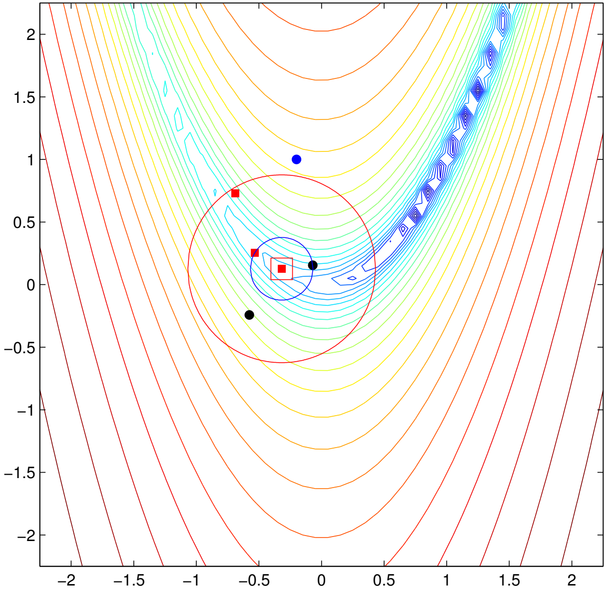

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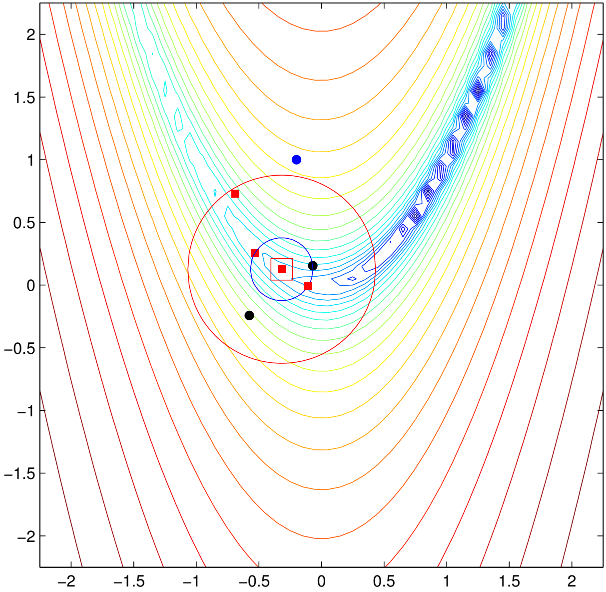

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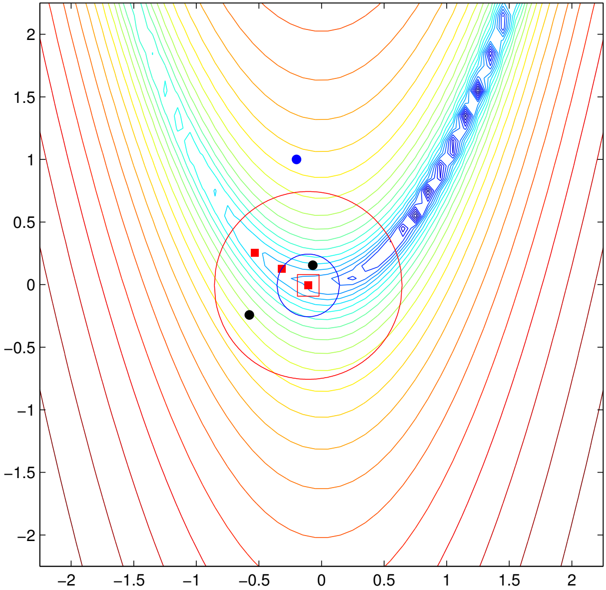

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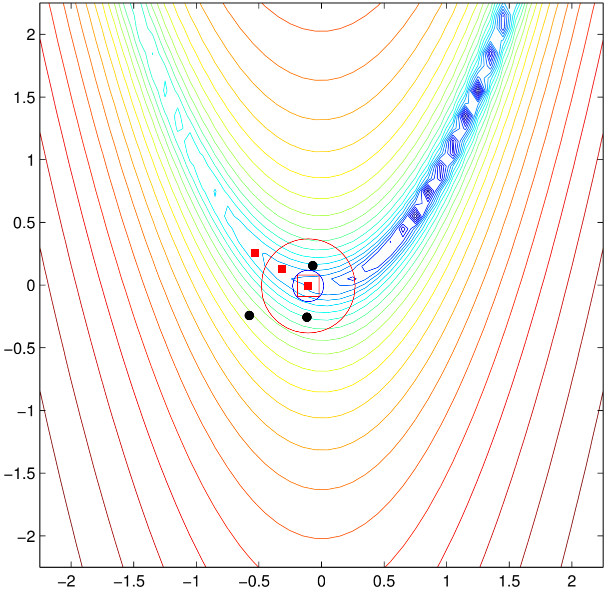

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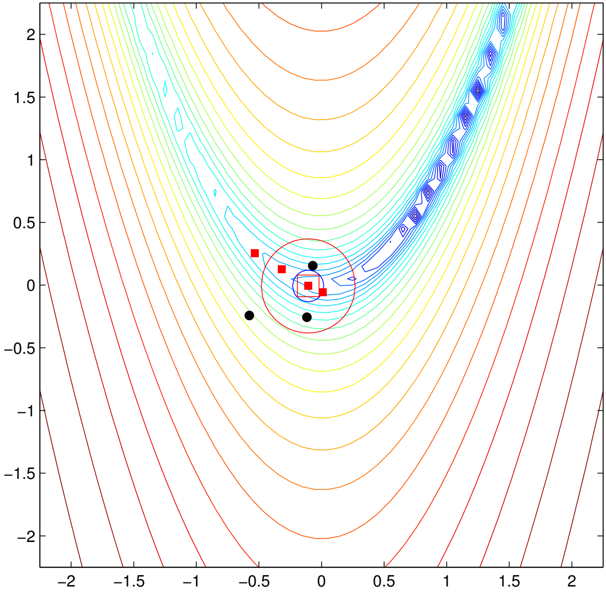

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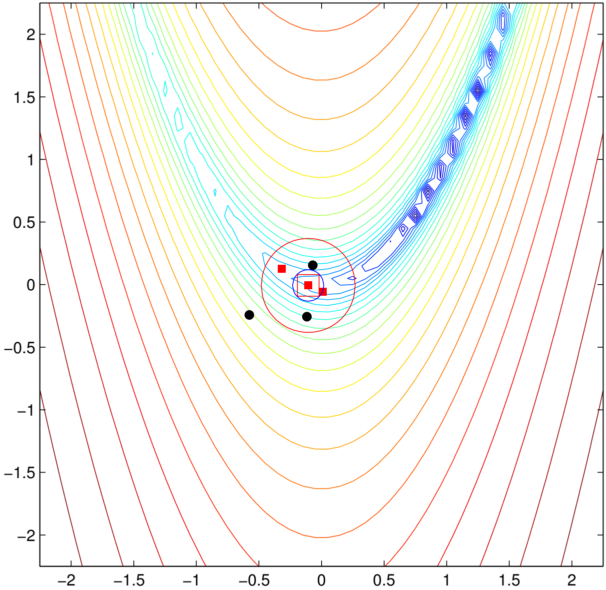
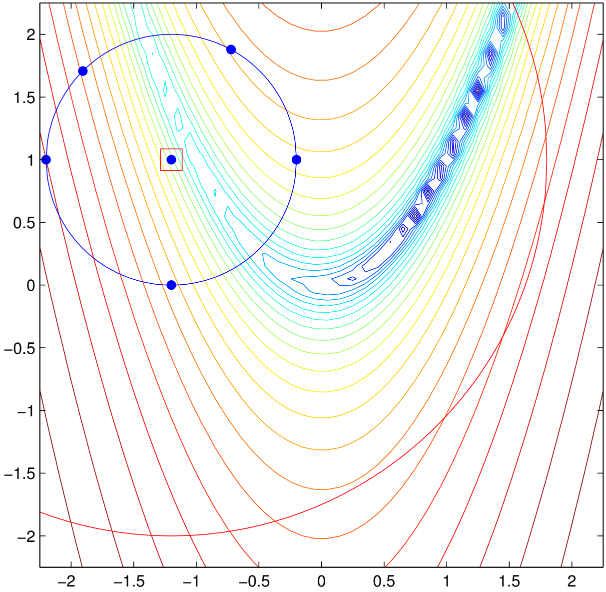


Model-based methods - Regression



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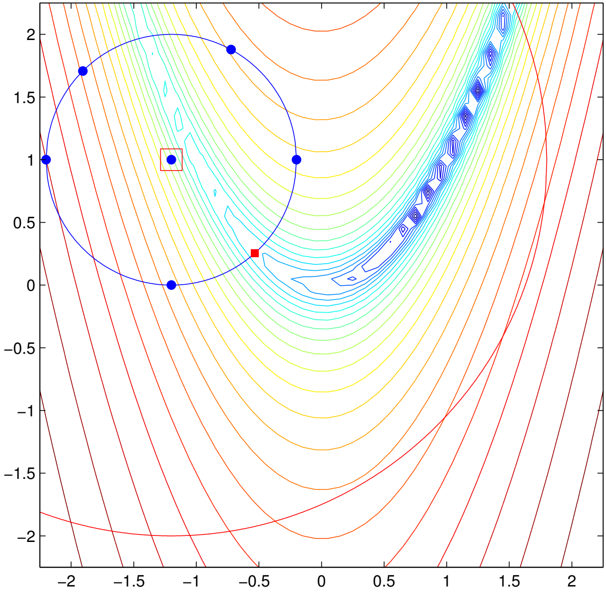

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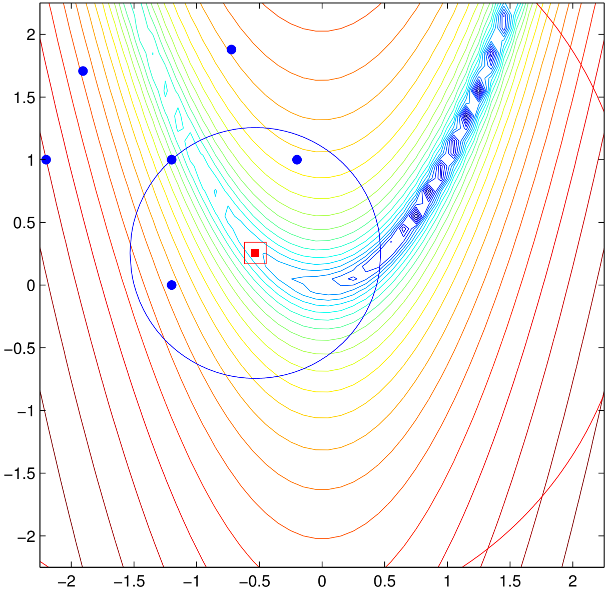

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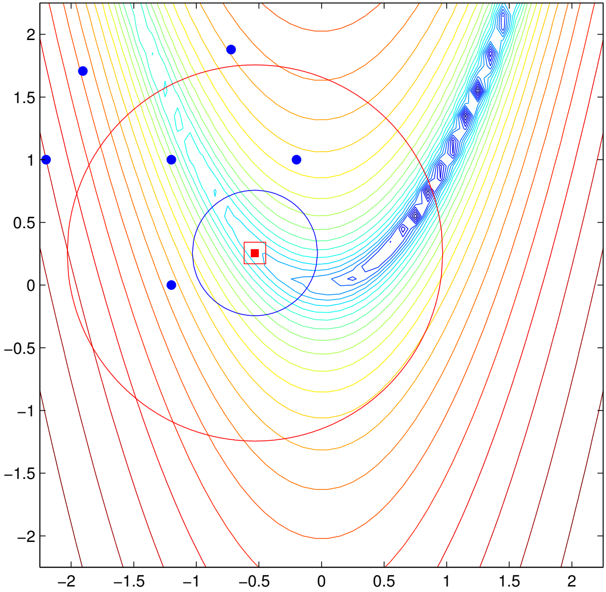

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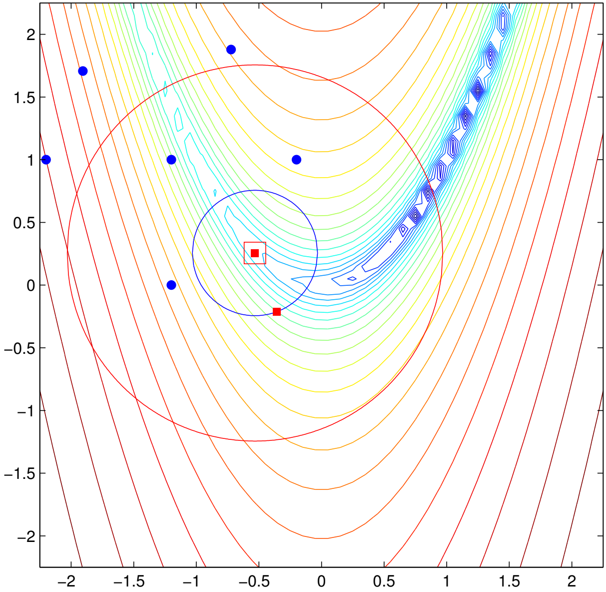

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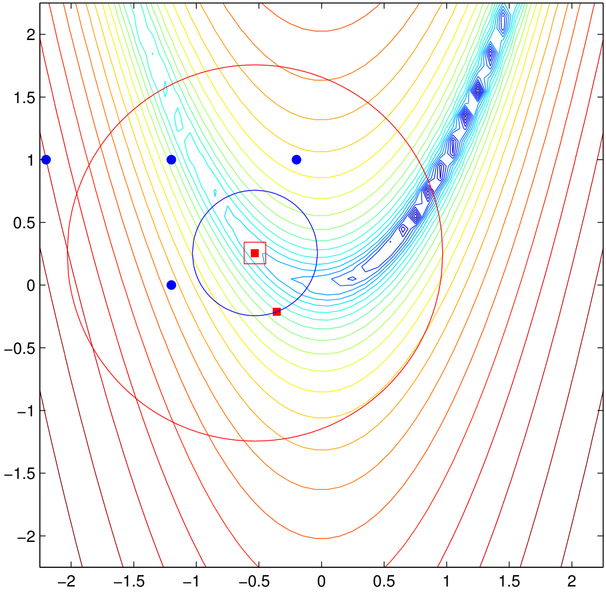

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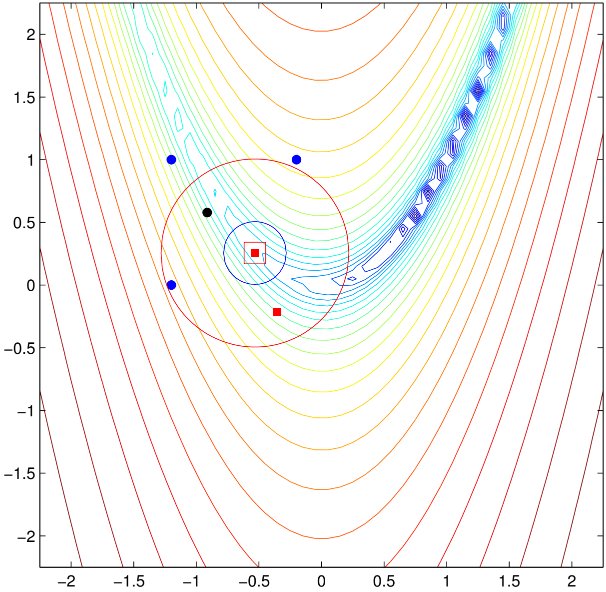

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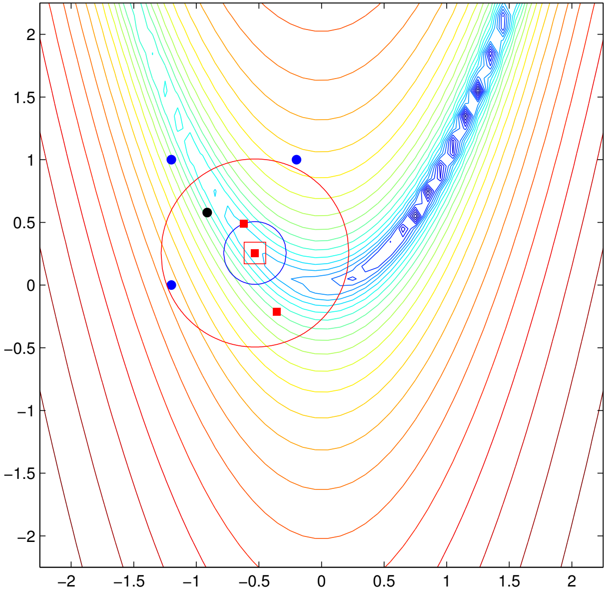

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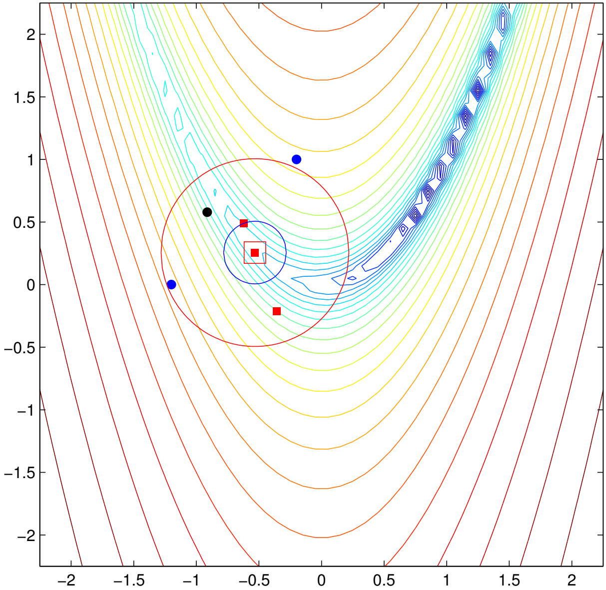

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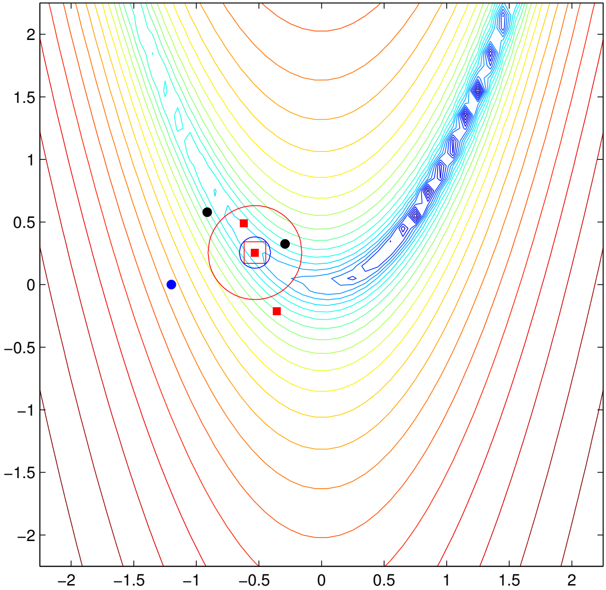

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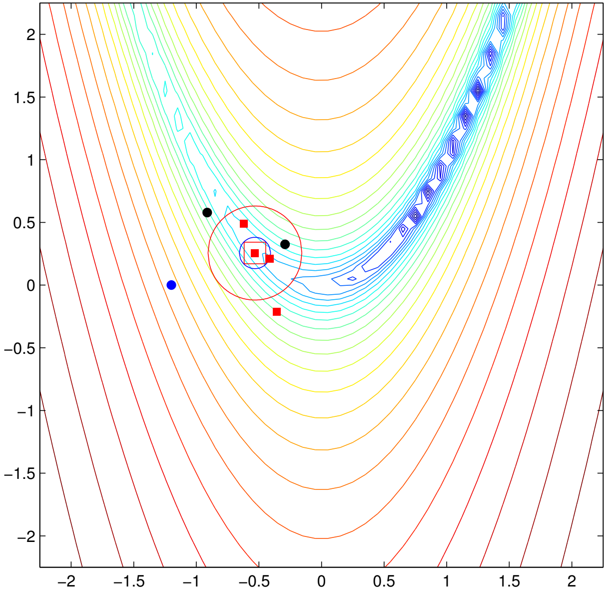

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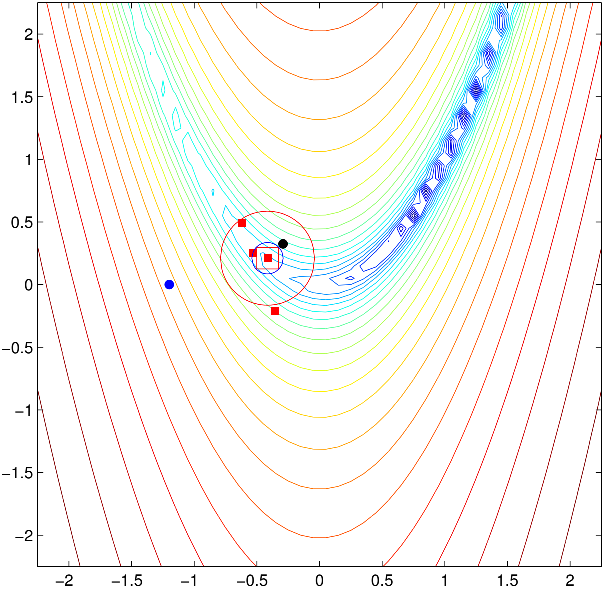

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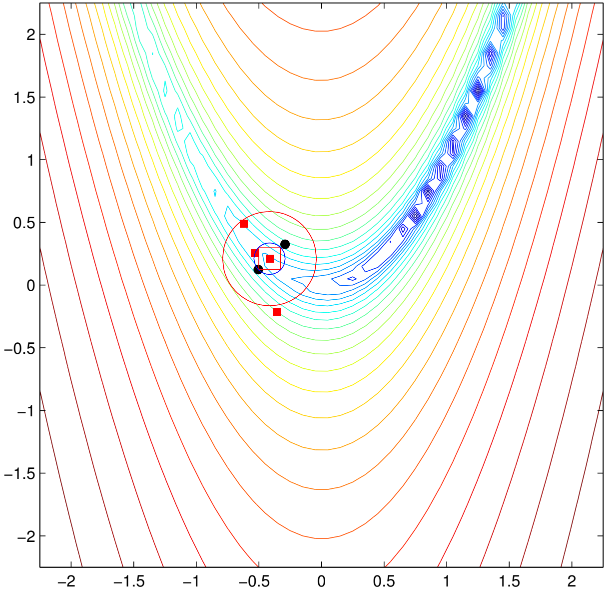

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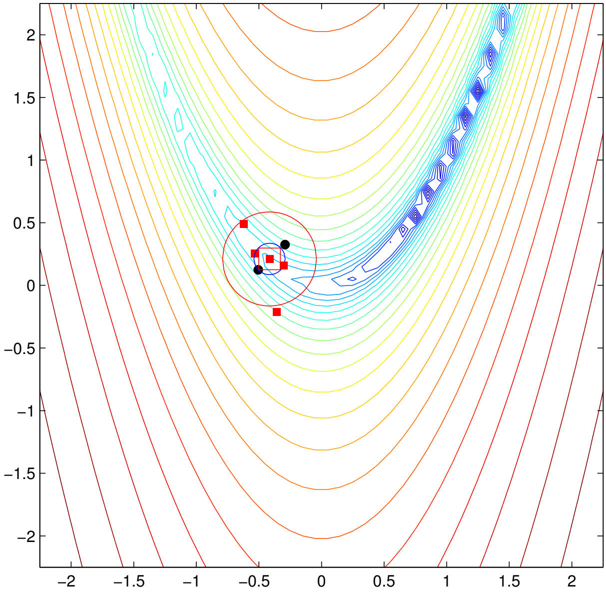

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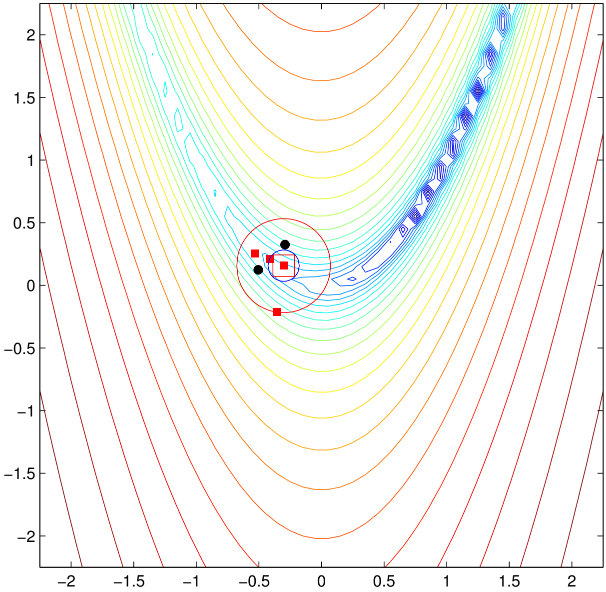

Other options

- Build a model of the entire space (Kriging)

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- Evolutionary algorithms
  - Simulated Annealing

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Other options

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  - Bee Colony Optimization

Other options

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  - Simulated Annealing
  - Ant Colony Optimization
  - Bee Colony Optimization
  - Particle Swarm

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  - Grey Wolf Optimization

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  - Particle Swarm
  - Cuckoo Search
  - Bacterial Colony Optimization
  - Grey Wolf Optimization
  - Firefly Optimization
  - Harmony Search
  - River Formation Dynamics

Problem Modifications

The Problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}}\; f(x)$$

subject to: $x \in \mathcal{D} = \{x : -\infty < l \leq x \leq u < \infty\}$

$\nabla f(x)$ **is not available**

Problem Modifications

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$$\nabla f(x) \ \ \text{is not available}$$

$$Ax \leq b$$

Problem Modifications

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$$\nabla f(x) \;\; \text{is not available}$$

$$c(x) \leq 0 \;\; (\nabla c(x) \text{ available})$$

Problem Modifications

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$c(x) \leq 0$ **(**$\nabla c(x)$ **unavailable)**

Problem Modifications

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$\nabla f(x)$ is not available

$s(x) \leq 0$ (but $s(x) > 0$ is less desirable)

Problem Modifications

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$\nabla f(x)$ is not available

$x \in \mathbb{Z}$

Problem Modifications

The Problem:

$$\underset{x\in\mathbb{R}^n}{\text{minimize}}\; f(x) = \tilde{f}(x) + \epsilon \quad \textbf{where} \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

subject to: $x \in \mathcal{D} = \{x : -\infty < l \leq x \leq u < \infty\}$

$\nabla f(x)$ **is not available**

Problem Modifications

The Problem:

$$\underset{x\in\mathbb{R}^n}{\text{minimize}}\; f(x) = \sum_{i=1}^{m} f_i(x)^2$$

subject to: $x \in \mathcal{D} = \{x : -\infty < l \leq x \leq u < \infty\}$

$\nabla f_i(x)$ **is not available**

Problem Modifications

The Problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; [f_1(x), f_2(x), \ldots, f_m(x)]$$

subject to: $x \in \mathcal{D} = \{x : -\infty < l \leq x \leq u < \infty\}$

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Problem Modifications

The Problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}}\ f(x)$$

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$\nabla f(x)$ **is not available**

Stochastic

Problem Formulation

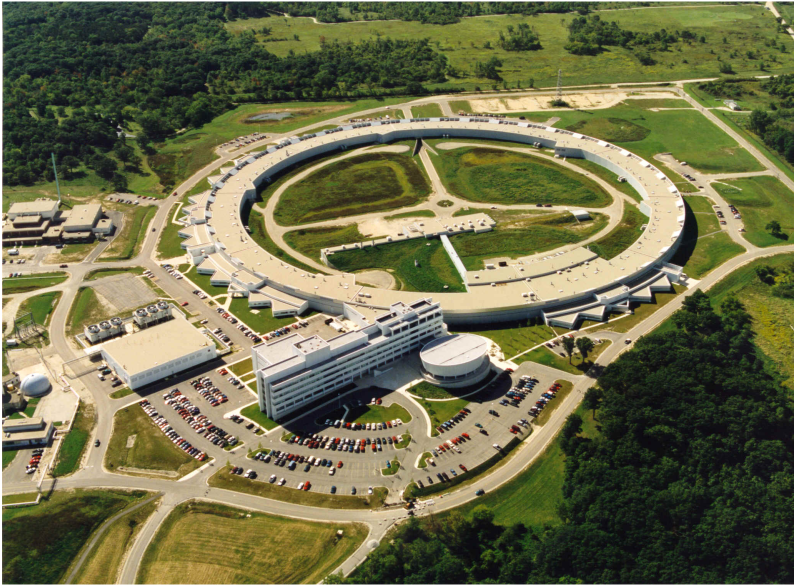
- We want to identify distinct local minimizers of the problem

$$\begin{aligned} \text{minimize}\, f(x) \\ l \le x \le u \\ x \in \mathbb{R}^n \end{aligned}$$

- The simulation f is already using parallel resources, but it does not scale to the entire machine.

- We do not expect hundreds of meaningful local minima.

Motivation



APS: $467M to build; tens of millions to operate.

Multi-Level Single Linkage

A multistart method with some local optimization routine $\mathcal{L}$:

Algorithm 1: MLSL

for $k = 1, 2, \ldots$ **do**

Evaluate f at N random points drawn uniformly from $\mathcal{D}$.

Start $\mathcal{L}$ at any previously evaluated point x:

- that is not a local minima
- $\nexists x_i : \|x - x_i\| \leq r_k$ and $f(x_i) < f(x)$

end

Multi-Level Single Linkage

If the simulation f, and local optimization method $\mathcal{L}$, and r_k satisfy some assumptions, then MLSL has nice theoretical properties.

- f
  - Twice continuously differentiable
  - All local minima are interior points
  - Some positive distance between all minima

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  - Strictly descent
  - Converges to nearby minimum (not stationary point)

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  - Twice continuously differentiable
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- $\mathcal{L}$
  - Strictly descent
  - Converges to nearby minimum (not stationary point)
- r_k

$$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \mathrm{vol}\left(\mathcal{D}\right) \frac{\sigma \log kN}{kN}} \tag{1}$$

Multi-Level Single Linkage

Theorem 8[1]

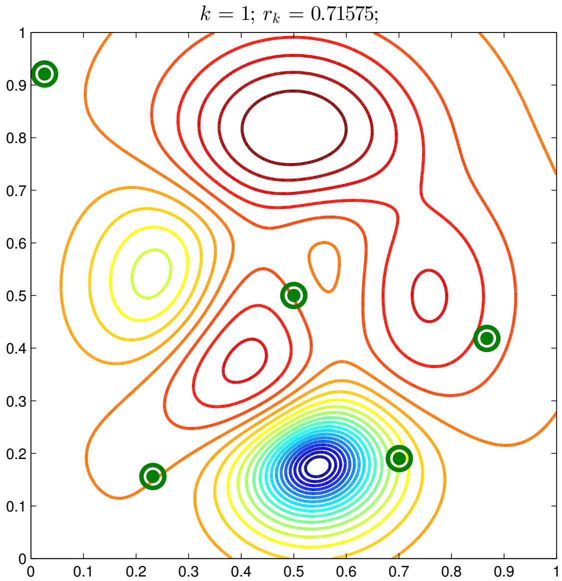
If r_k is defined by (1) and $\sigma > 2$, then the probability that $\mathcal{L}$ is started at iteration k tends to 0 with increasing k.
If $\sigma > 4$, then, even if the sampling continues forever, the total number of local searches ever started is finite with probability 1.

Theorem 12[1]

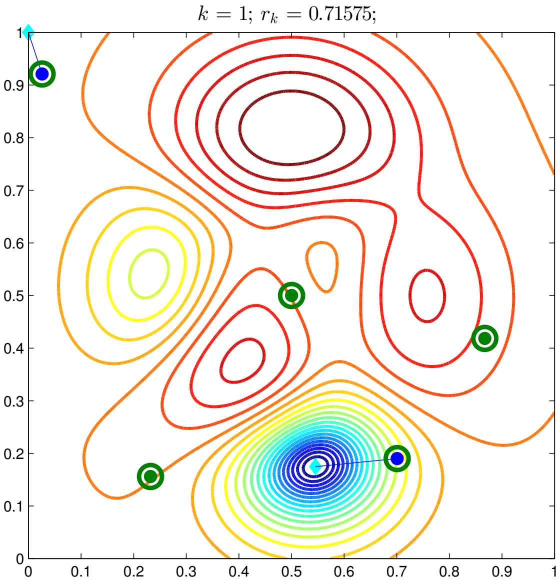
If $r_k \to 0$, all local minima will be found.

[1] A. H. G. Rinnooy Kan and G. T. Timmer. "Stochastic Global Optimization Methods Part II: Multi Level Methods." *Mathematical Programming*, 39(1):57–78, Sept. 1987.

Multi-Level Single Linkage



Multi-Level Single Linkage



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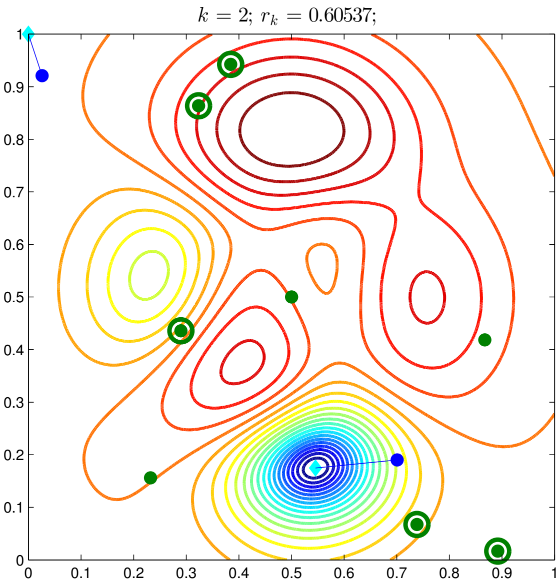
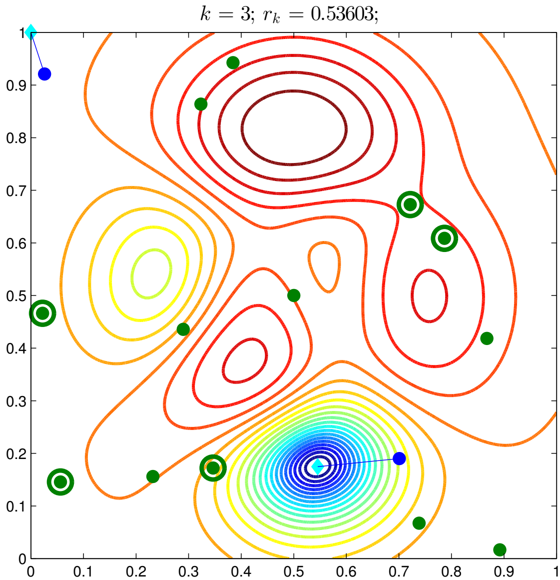
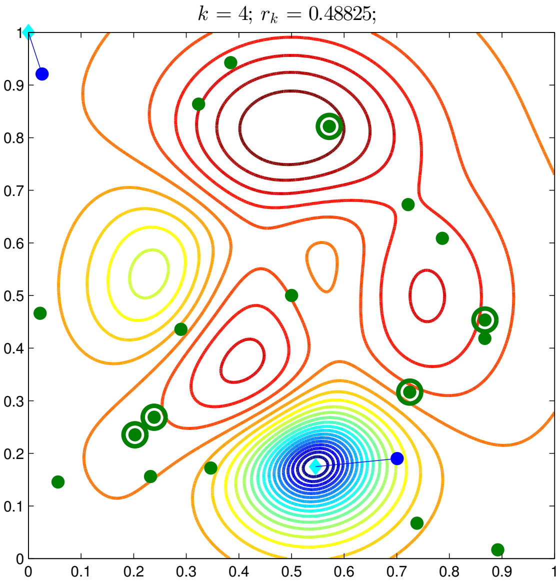


Multi-Level Single Linkage



Multi-Level Single Linkage



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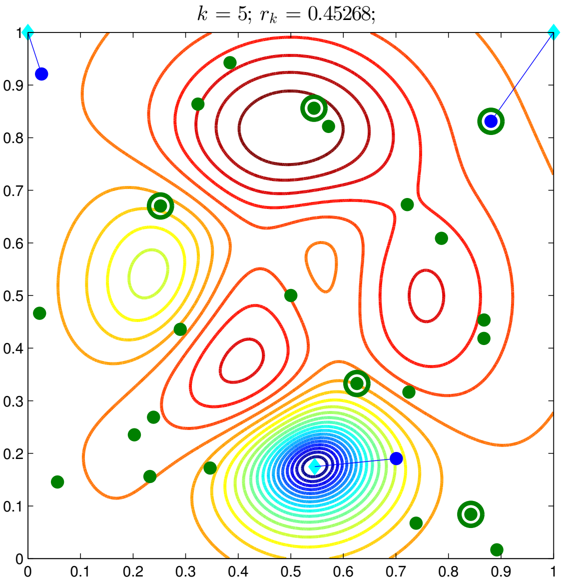

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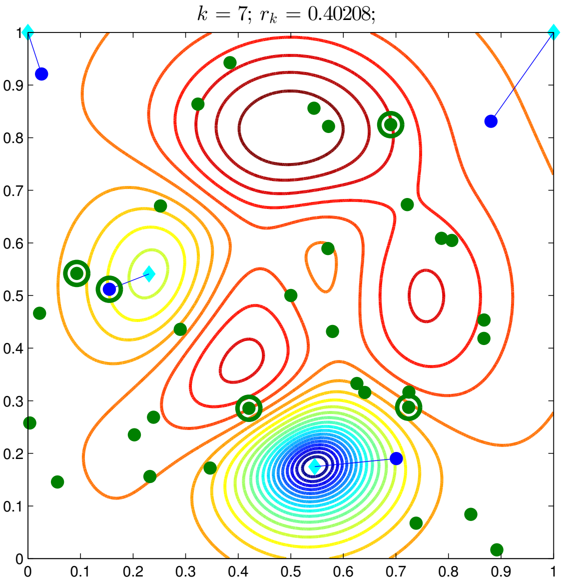

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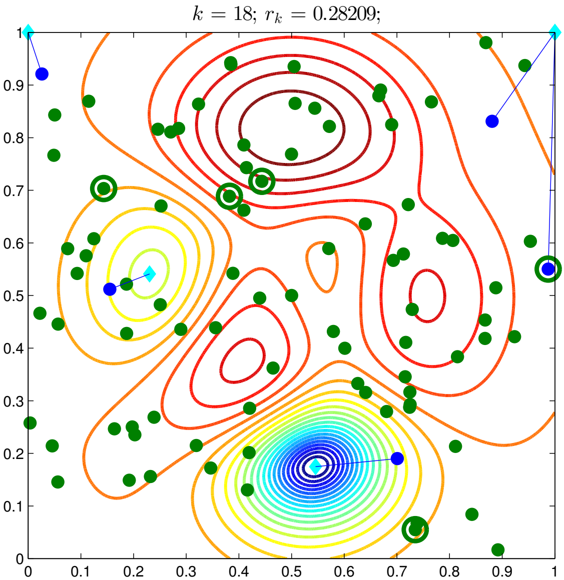

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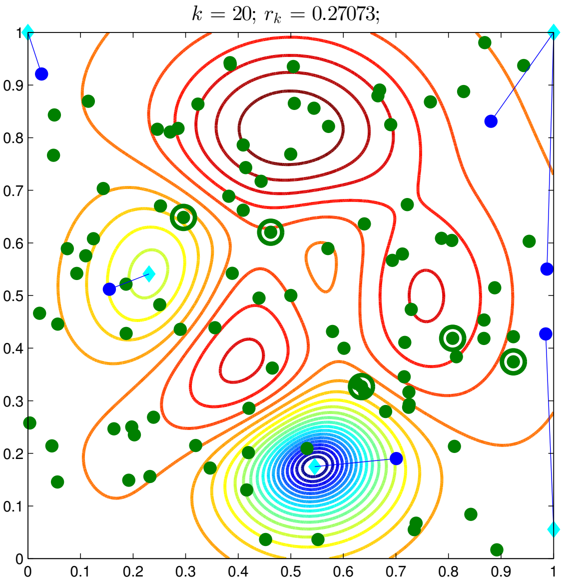
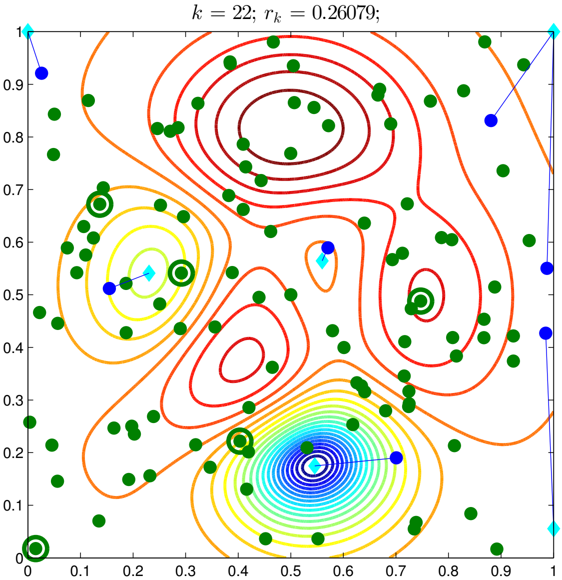
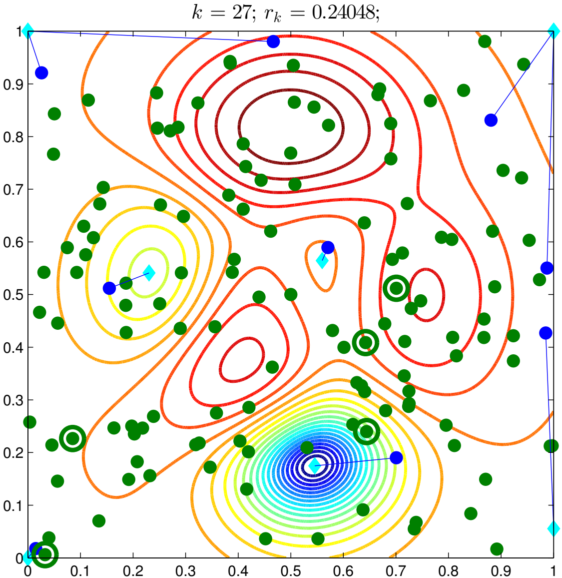


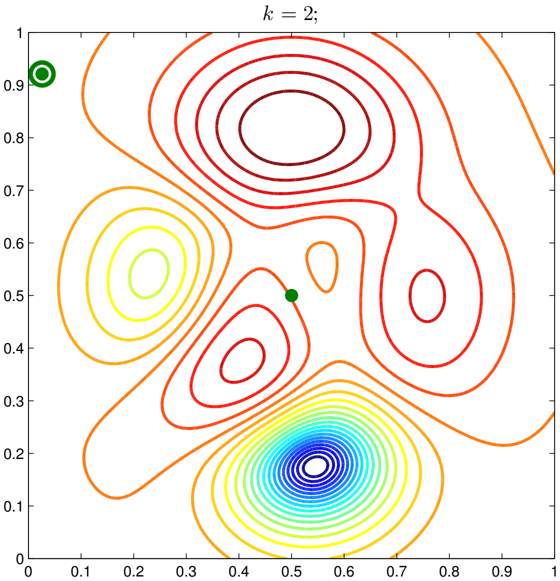
Multi-Level Single Linkage



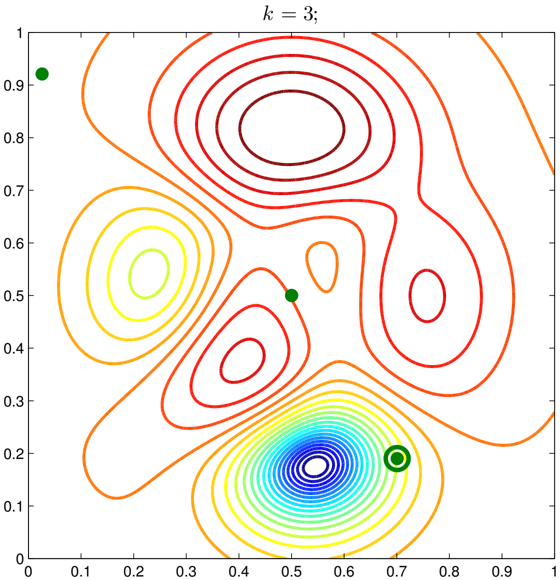
Multi-Level Single Linkage



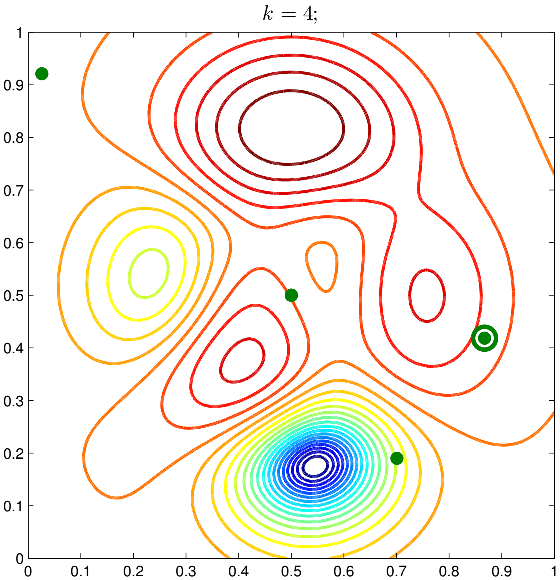
Derivative-free MLSL



Derivative-free MLSL



Derivative-free MLSL



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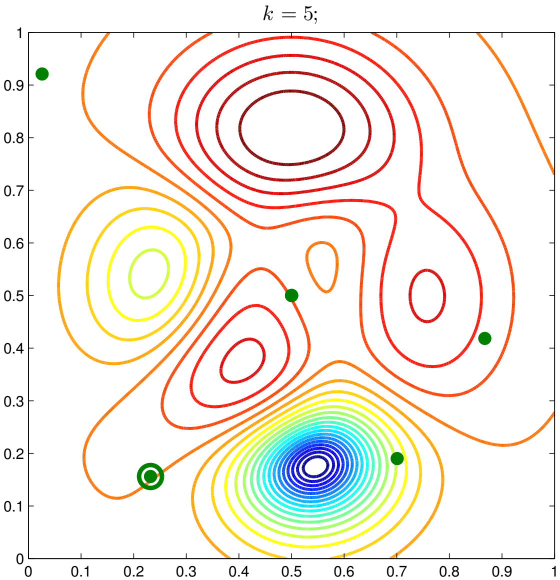

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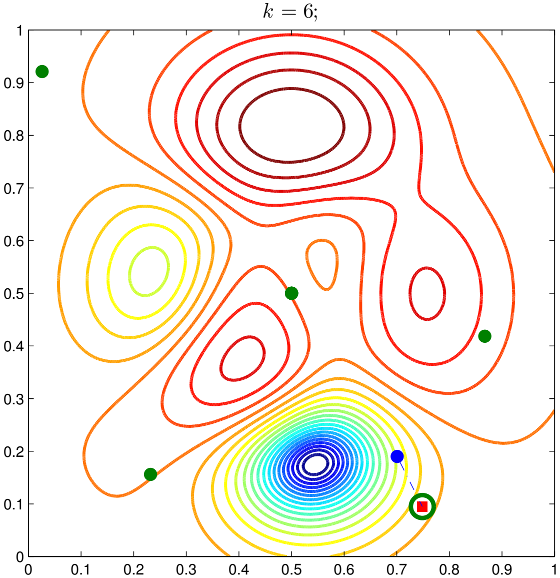

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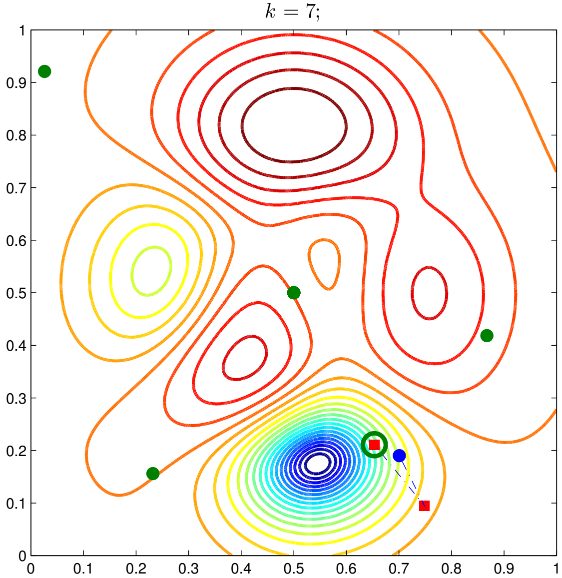

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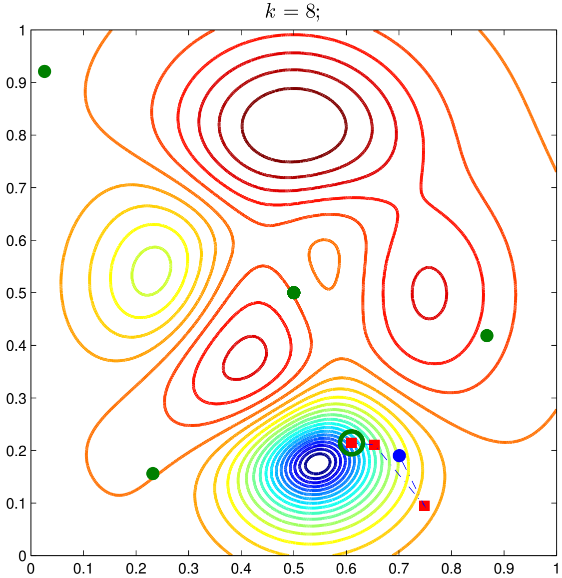

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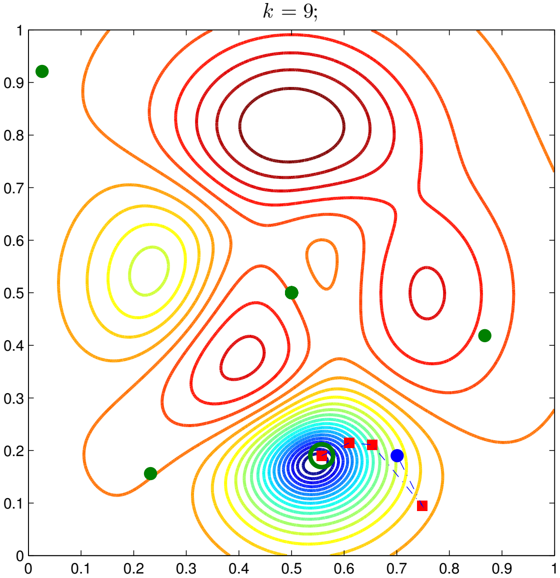

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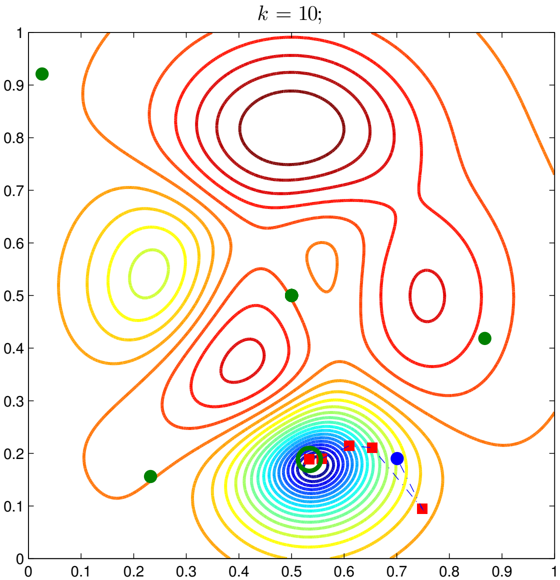

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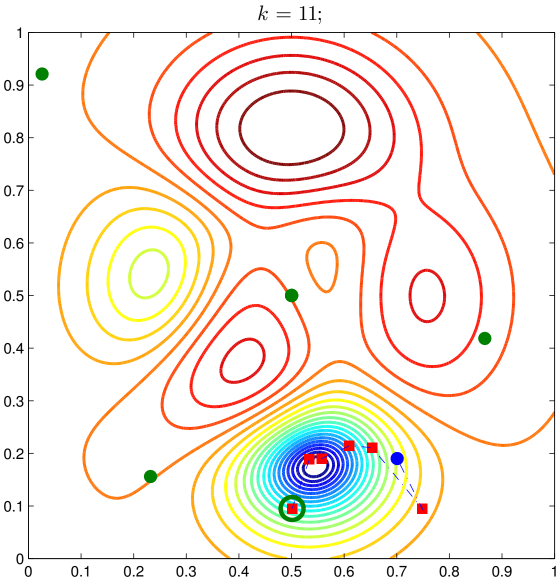

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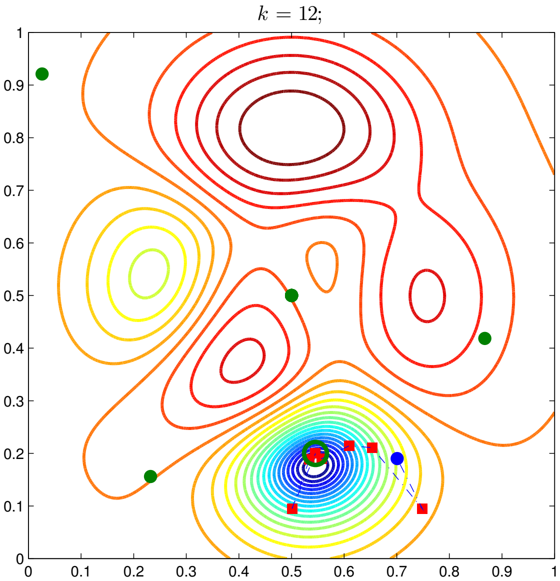

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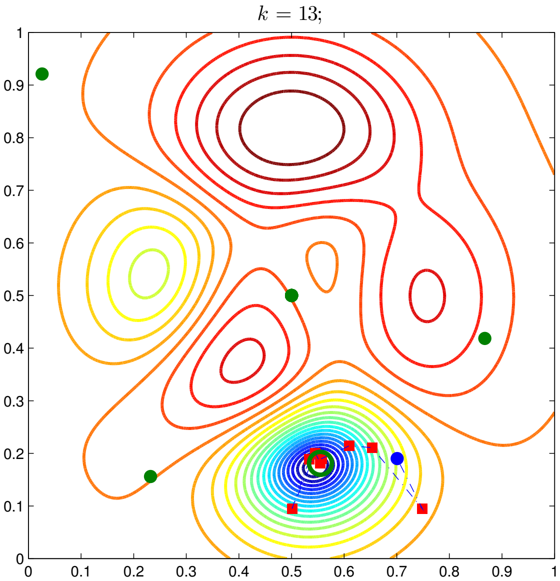

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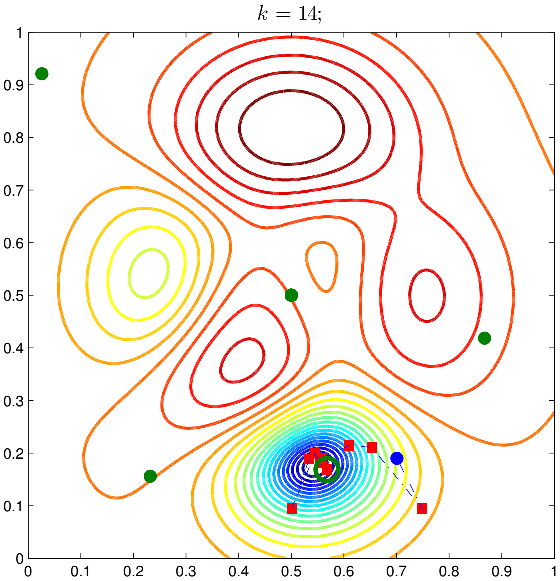

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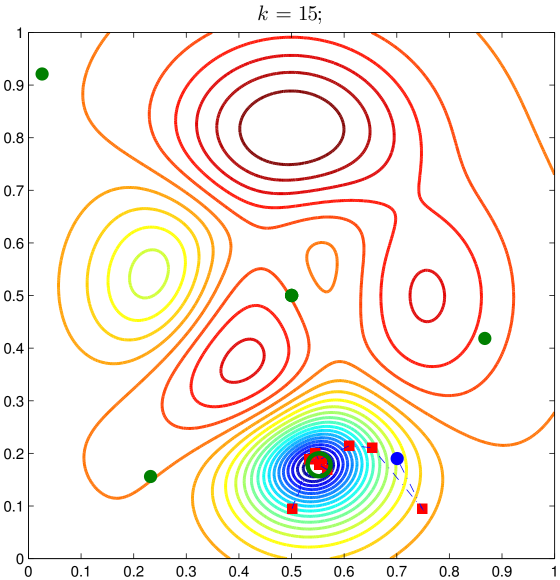

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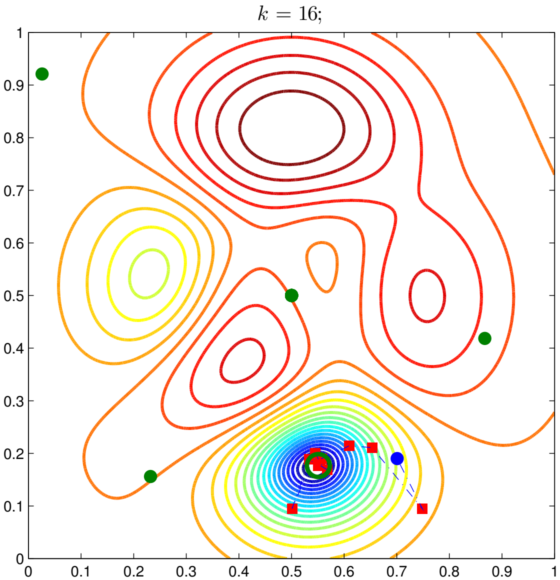

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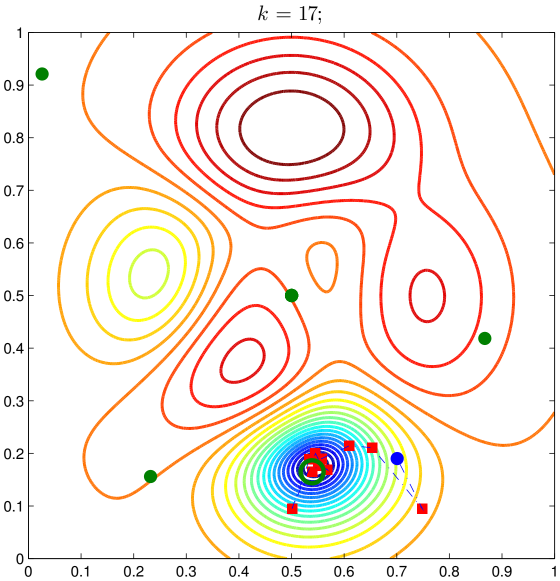

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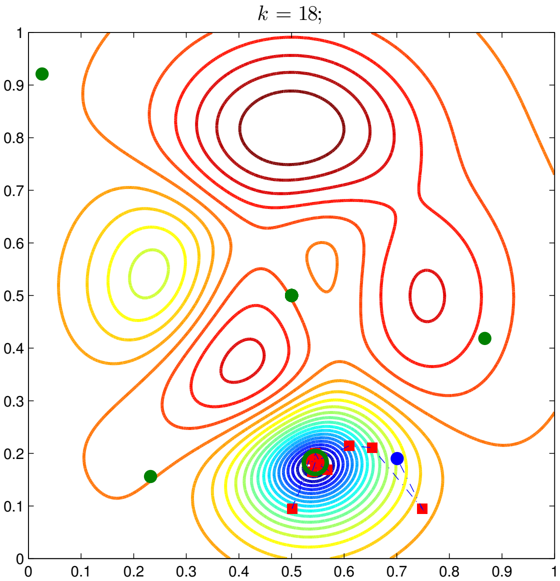

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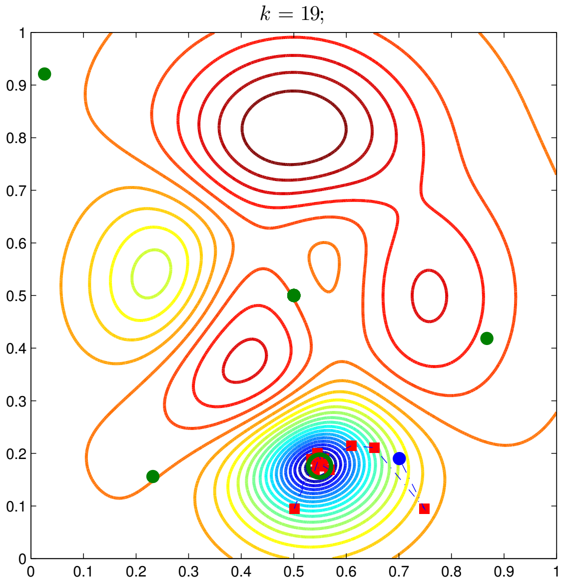

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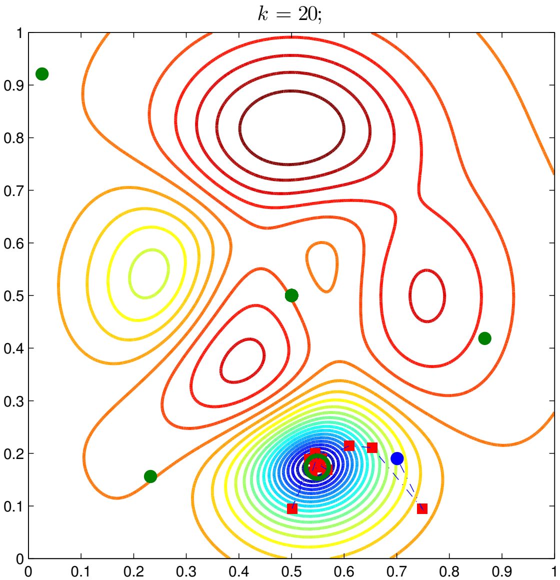

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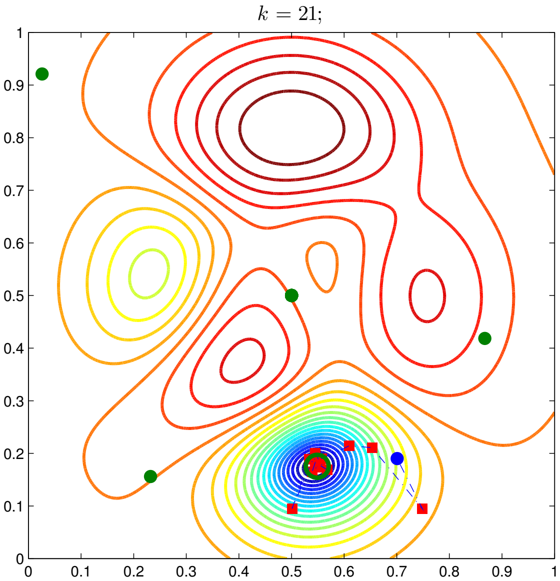

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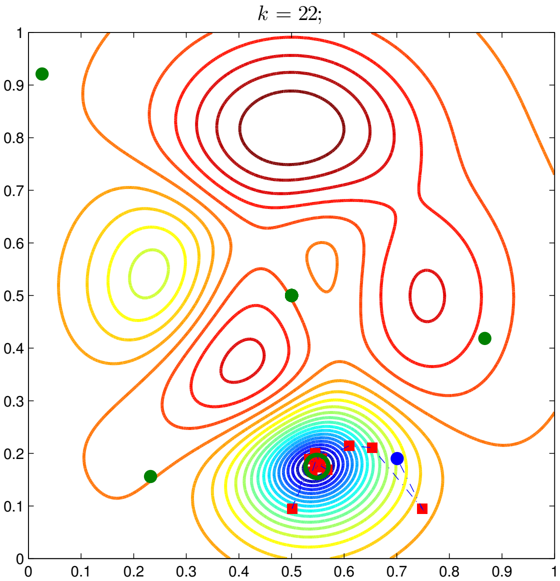

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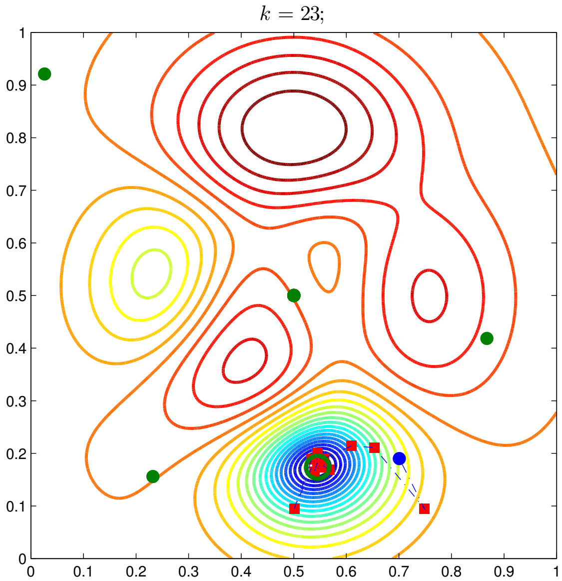

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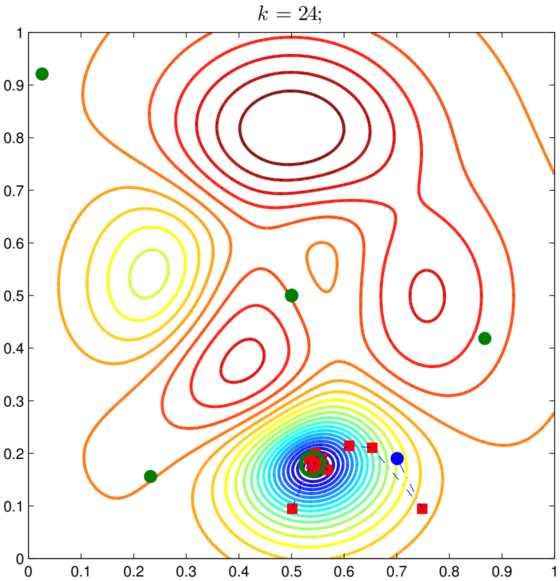

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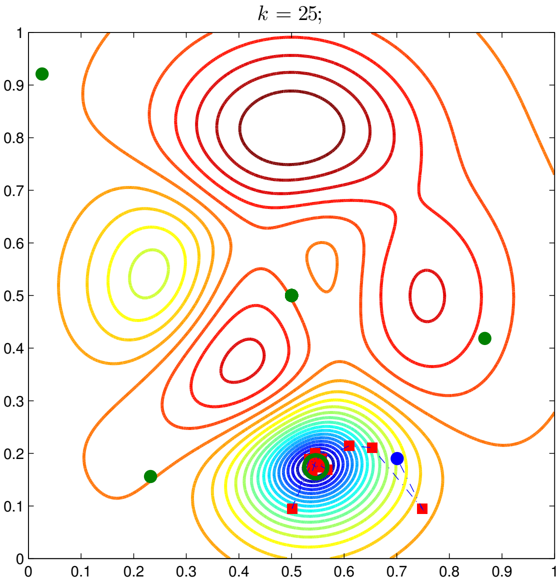

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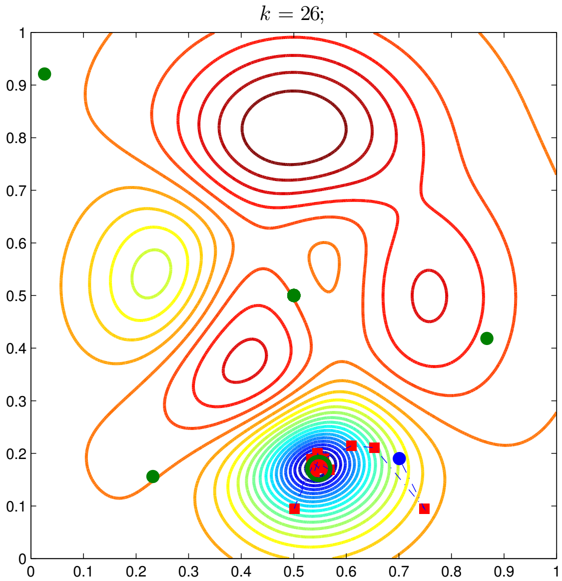

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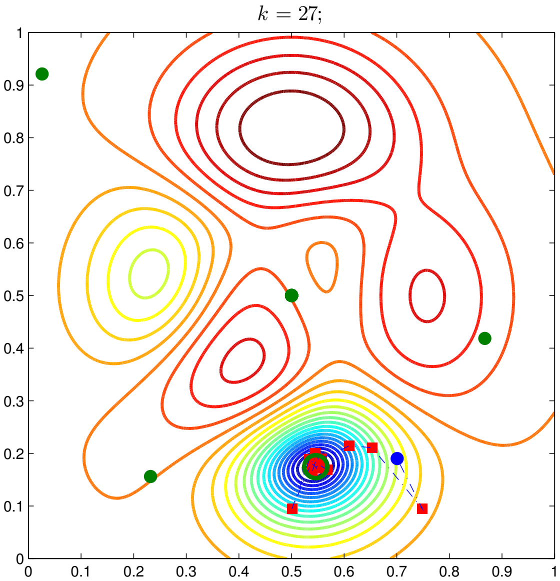

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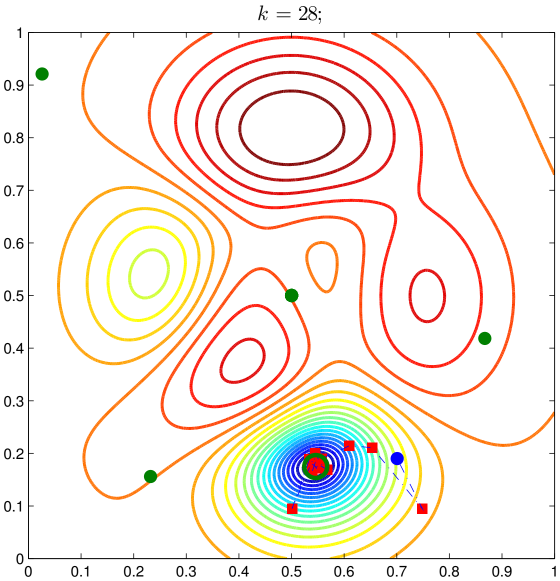

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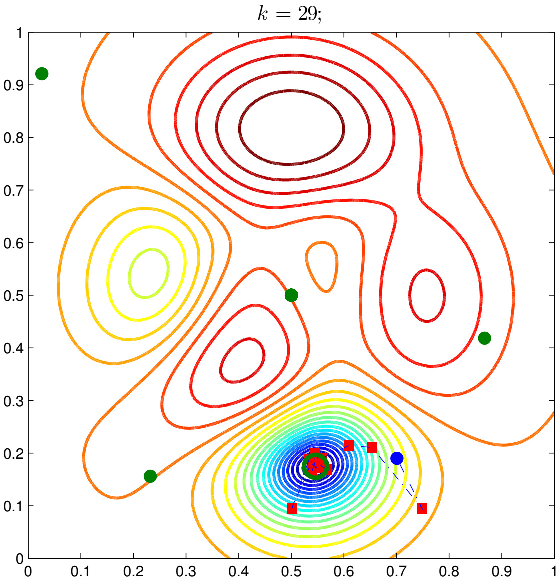

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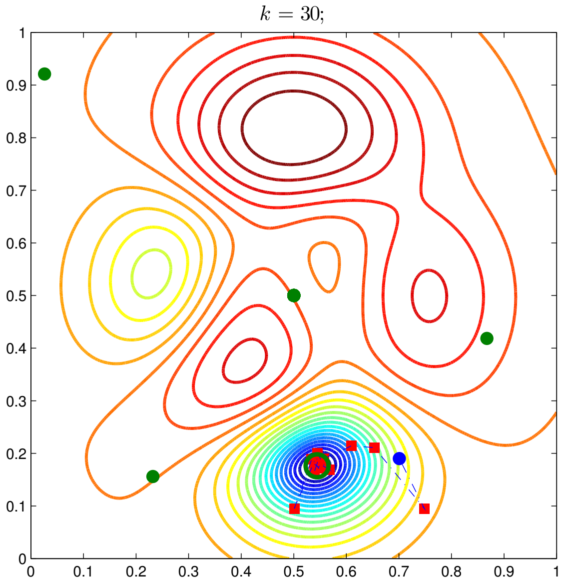

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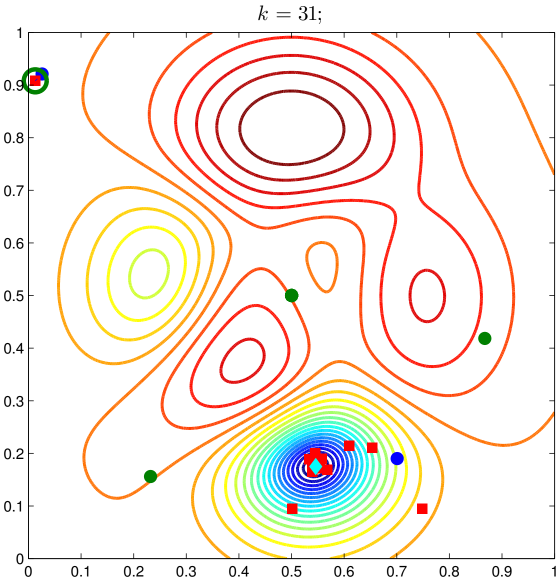

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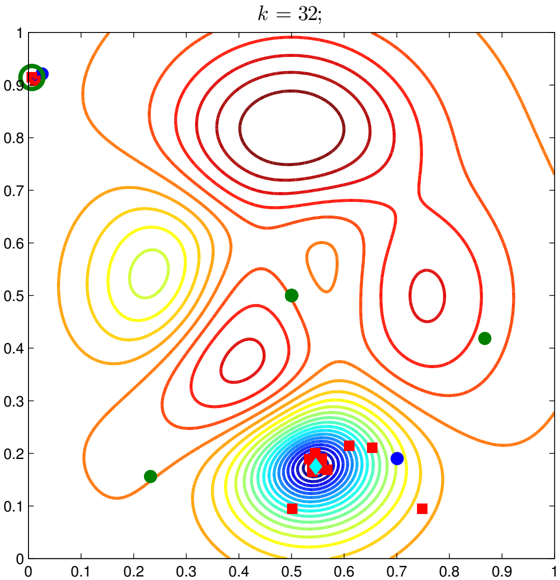
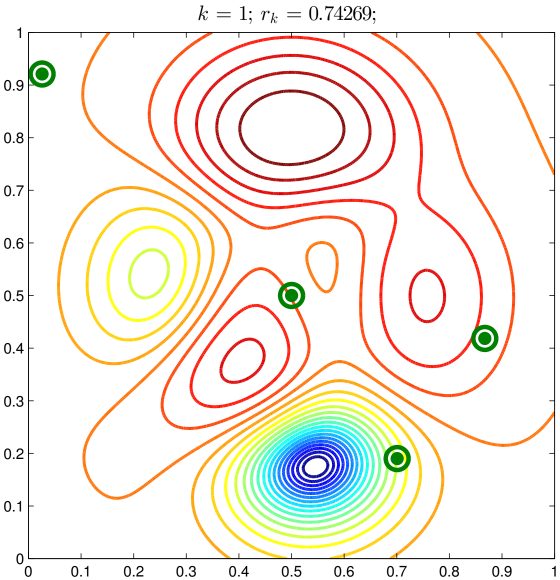


Derivative-free MLSL

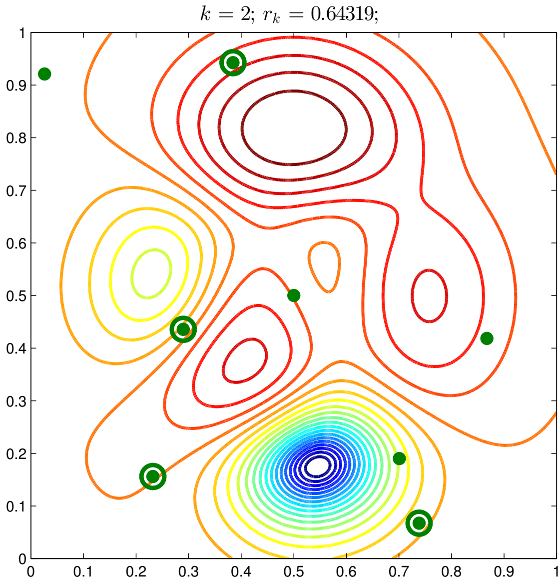
- If we had the ability to concurrently evaluate points, what might be the best course?

- Is it better to do finite-difference computations or separate local optimization runs?

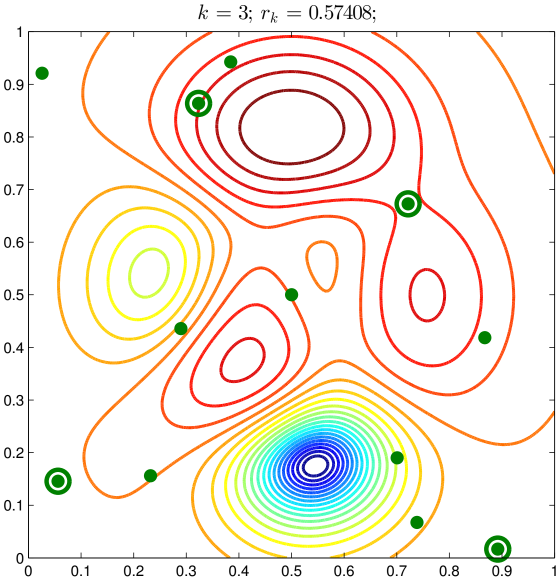
Our Method



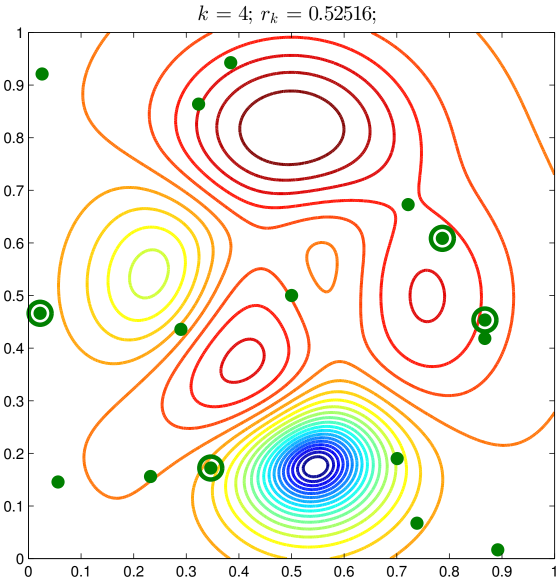
Our Method



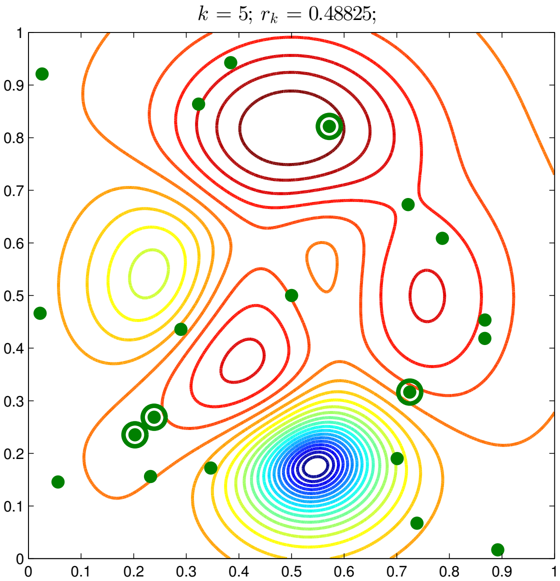
Our Method



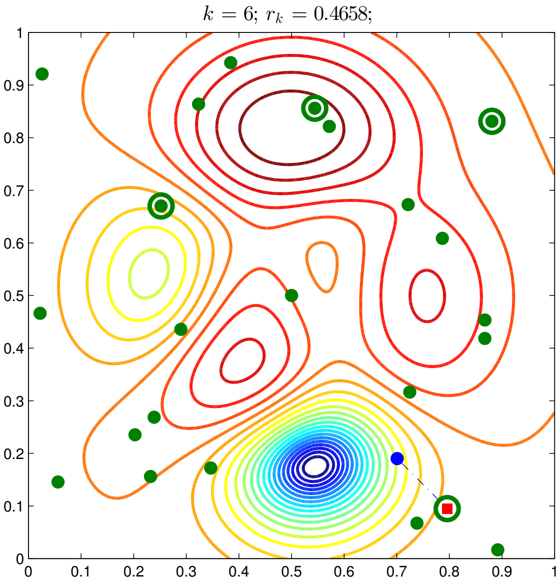
Our Method



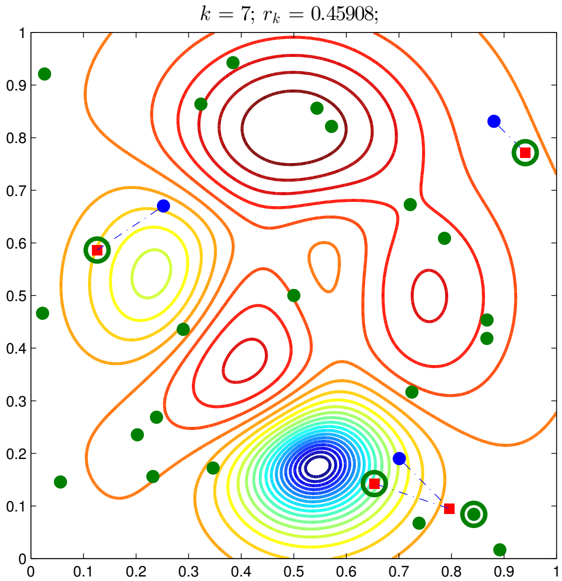
Our Method



Our Method

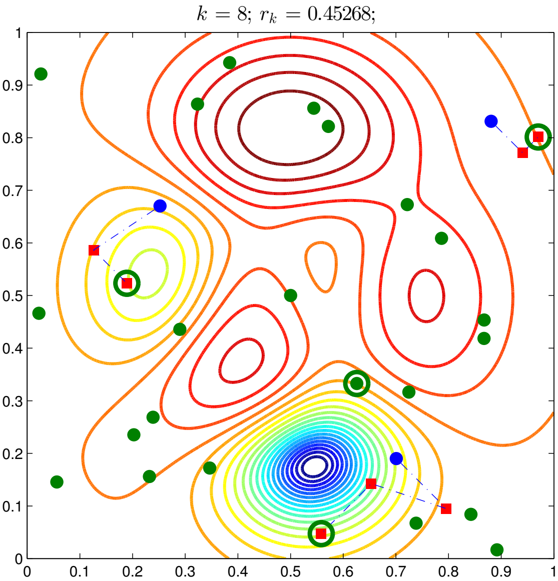


Our Method

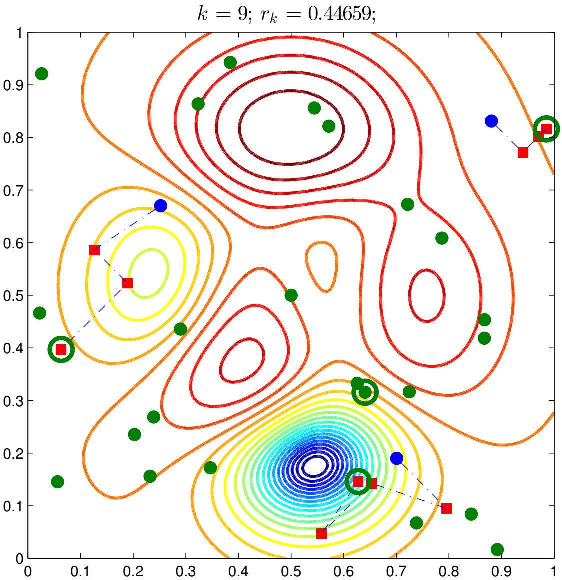


$k = 7;\ r_k = 0.45908;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1

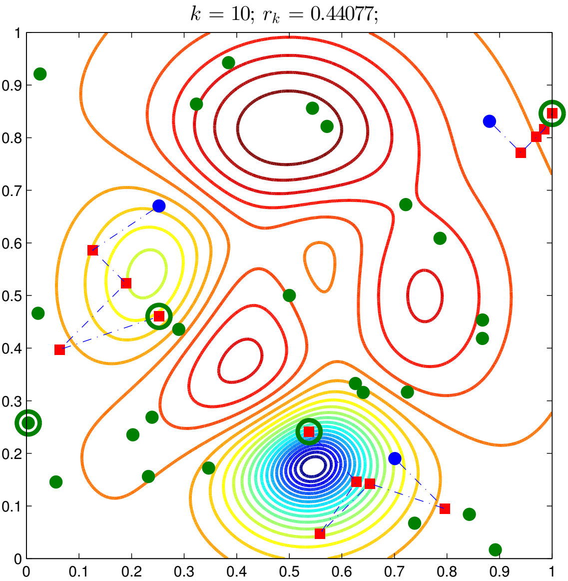
Our Method



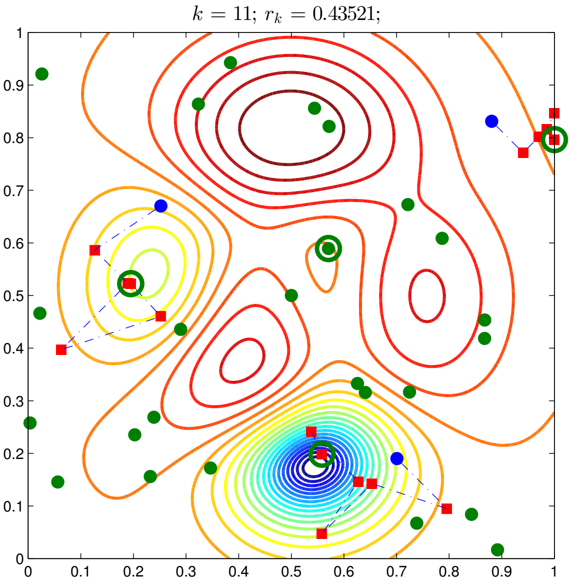
Our Method



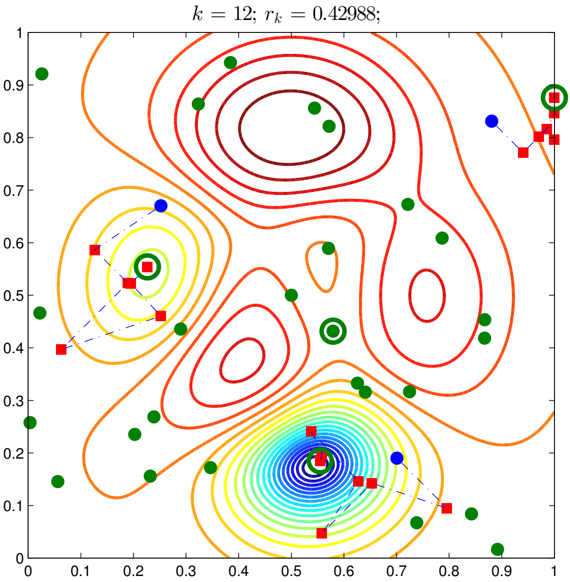
Our Method



Our Method

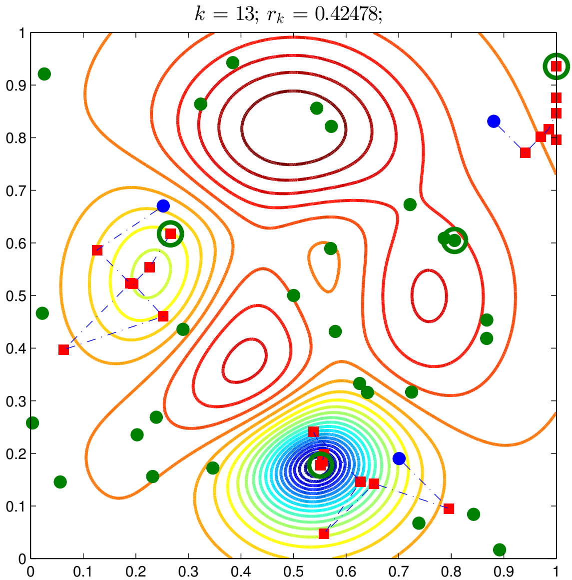


Our Method

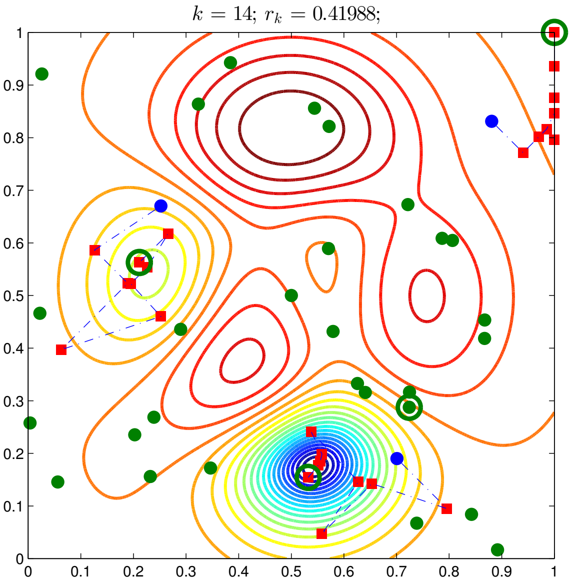


$k = 12;\ r_k = 0.42988;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1

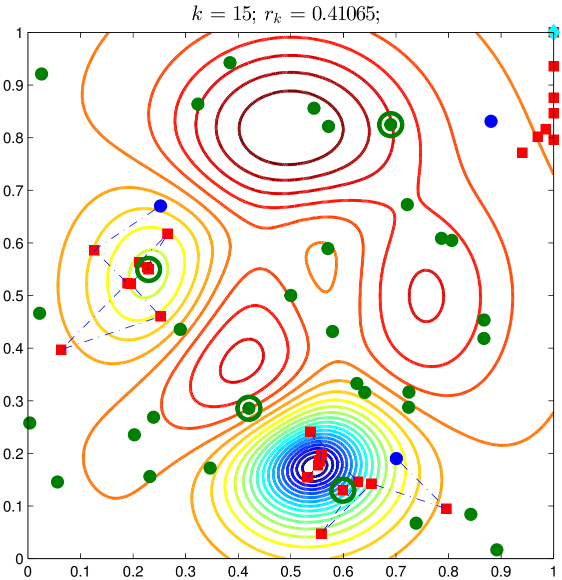
Our Method



Our Method

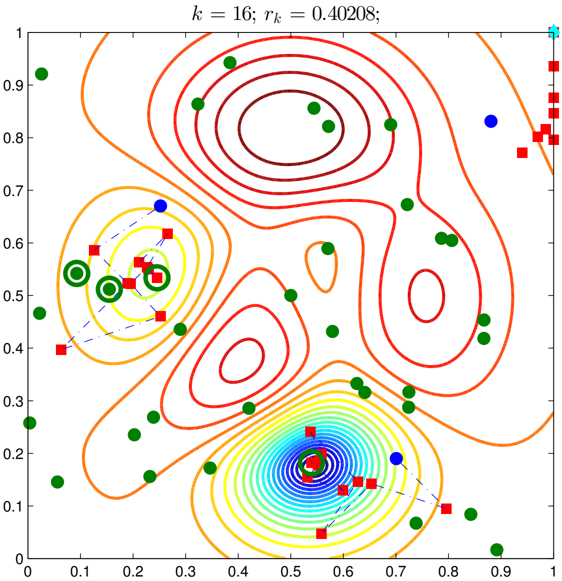


Our Method

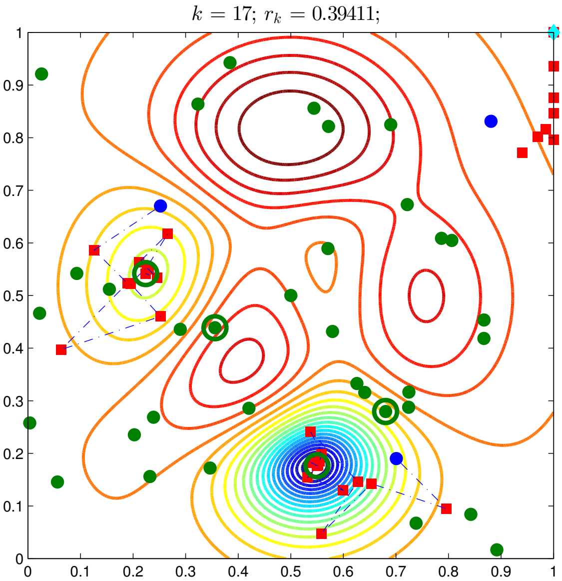


$k = 15;\ r_k = 0.41065;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

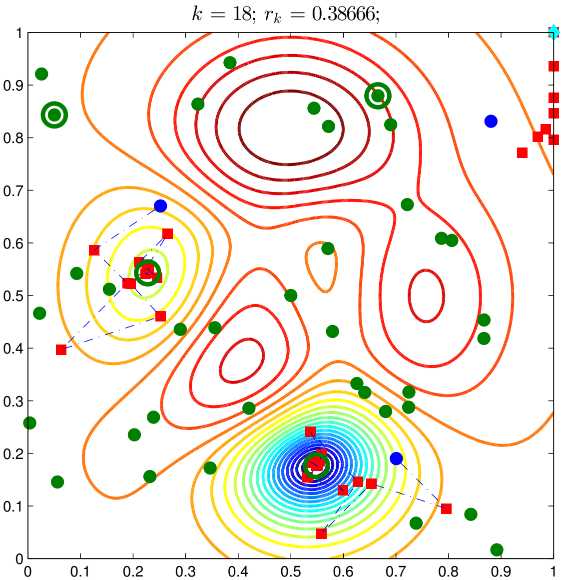
Our Method



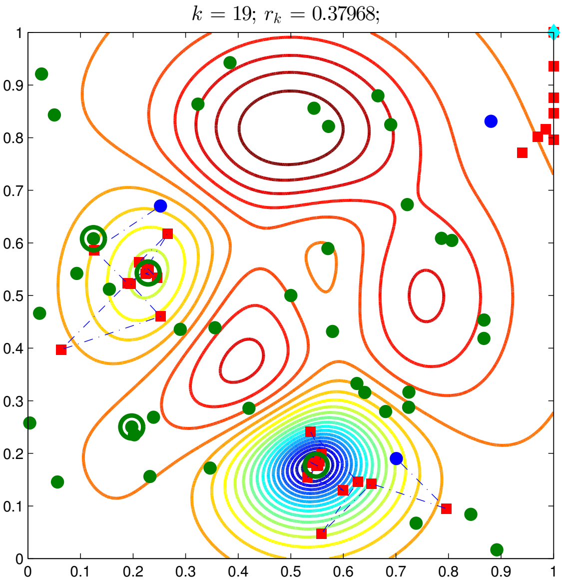
Our Method



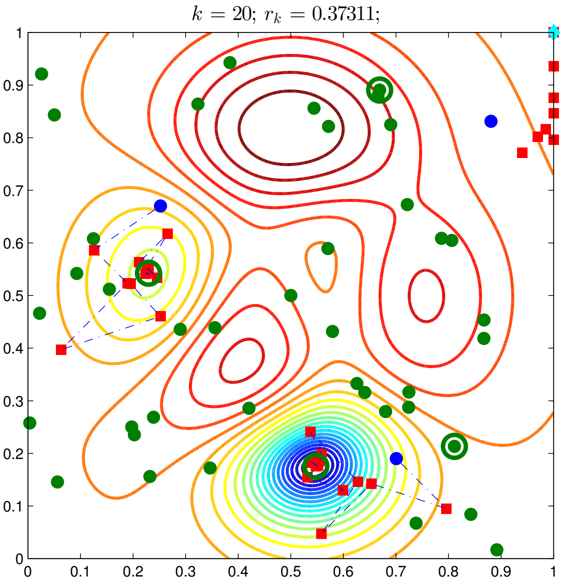
Our Method



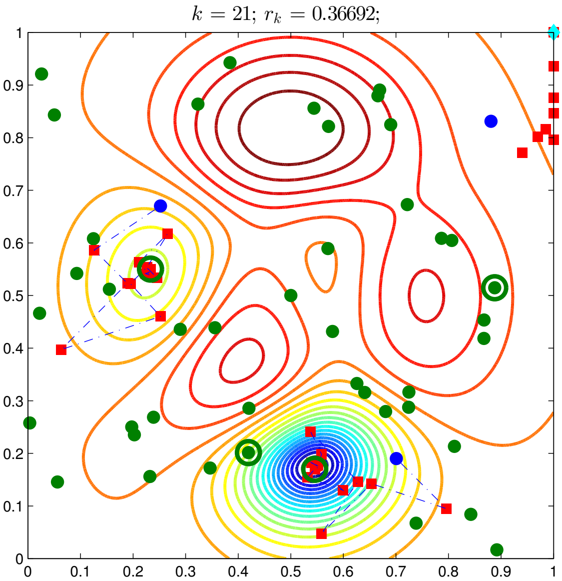
Our Method



Our Method

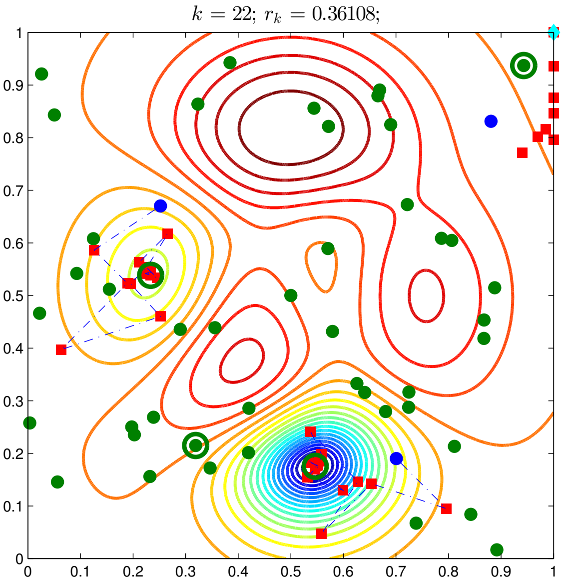


Our Method

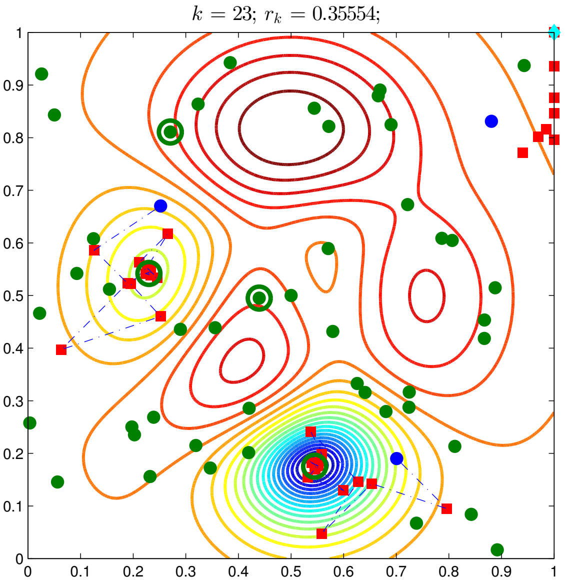


$k = 21;\ r_k = 0.36692;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

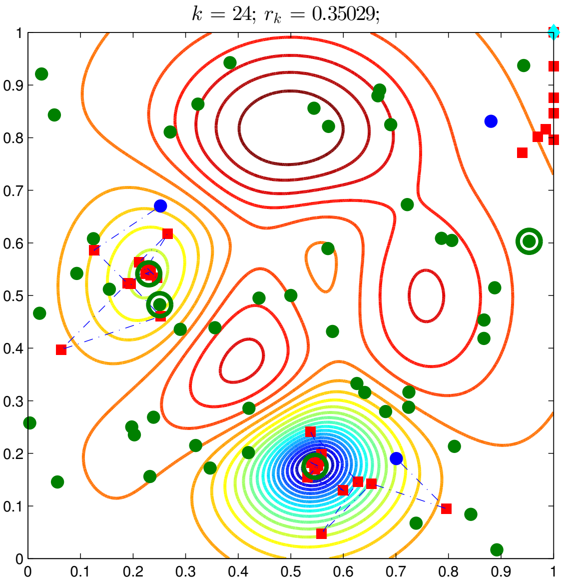
Our Method



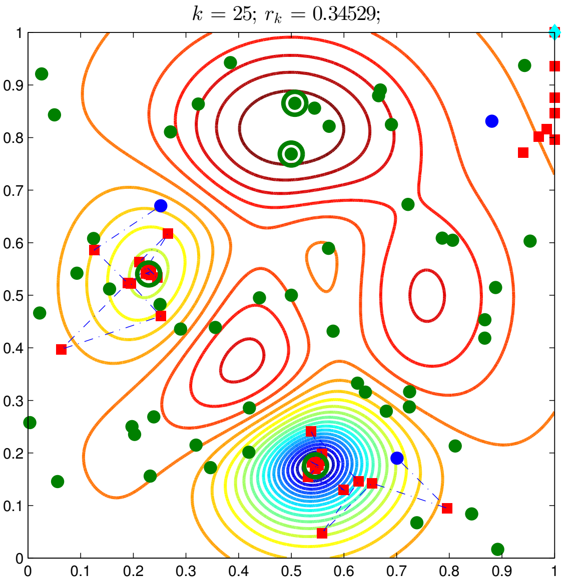
Our Method



Our Method



Our Method



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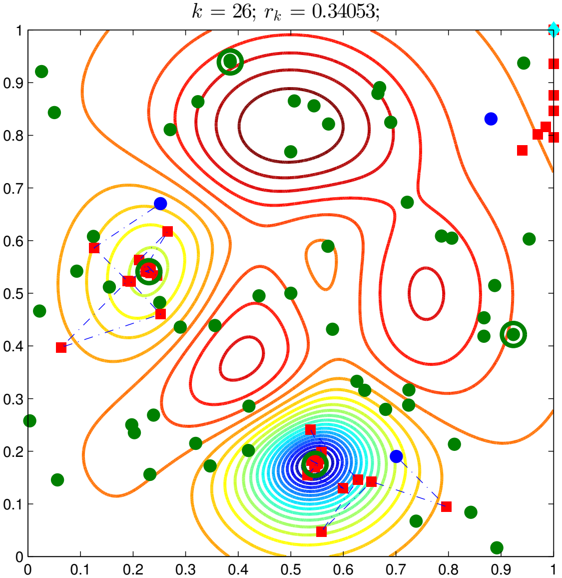
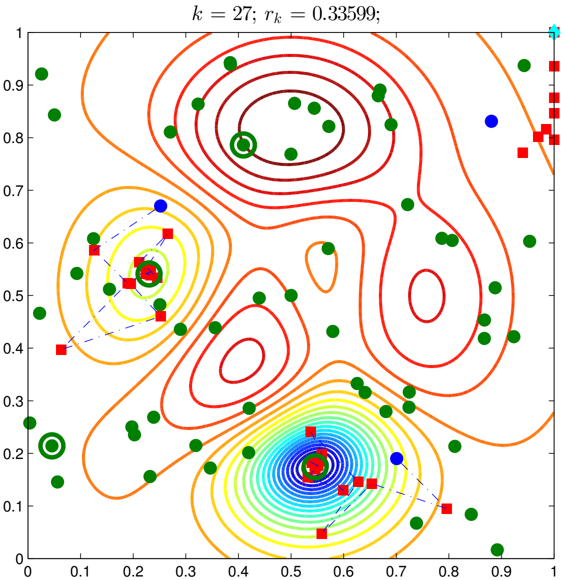
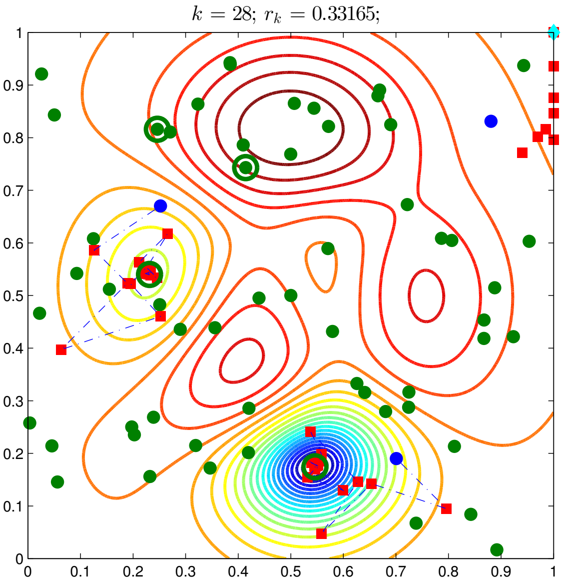


Our Method



Our Method



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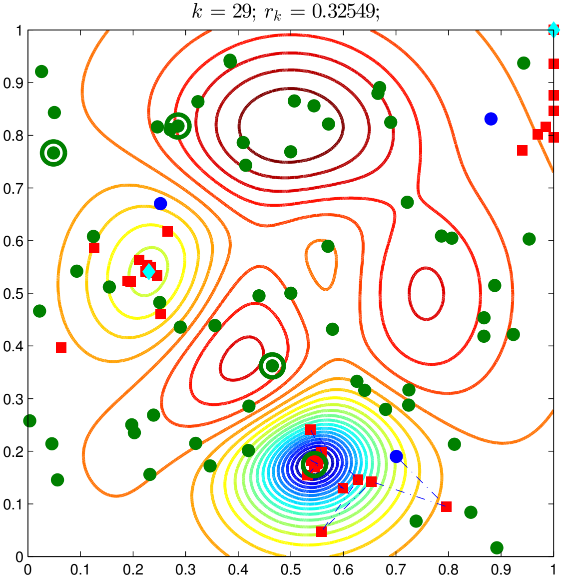

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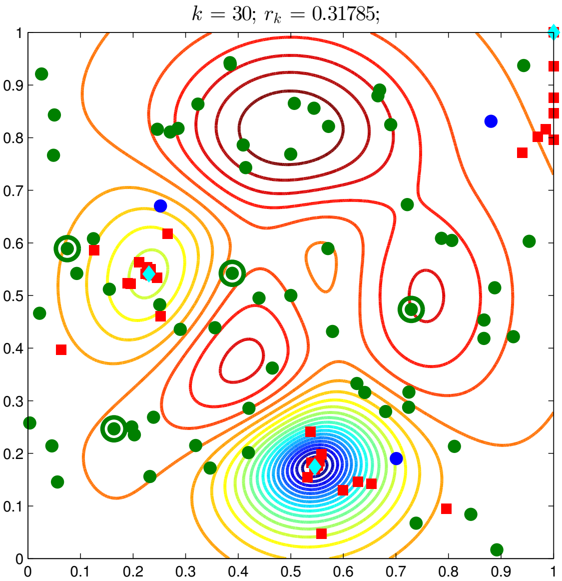
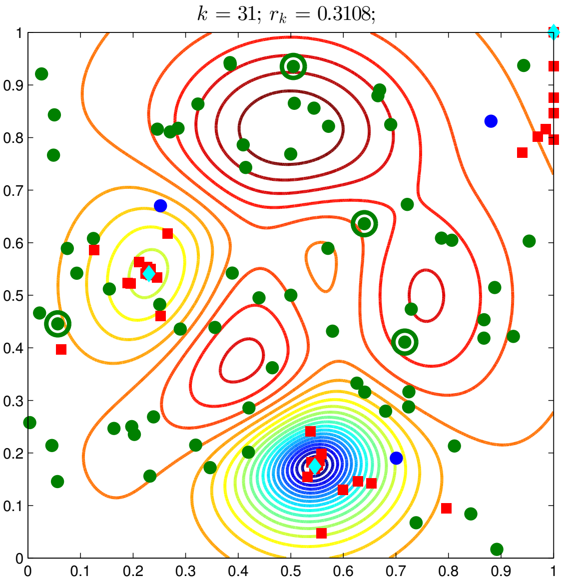
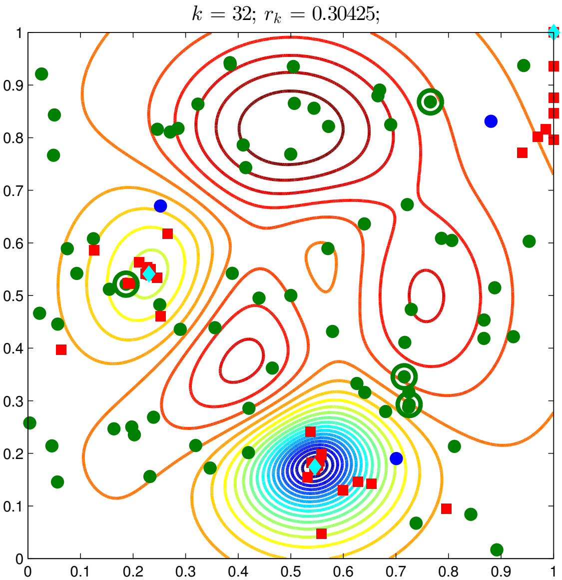


Our Method

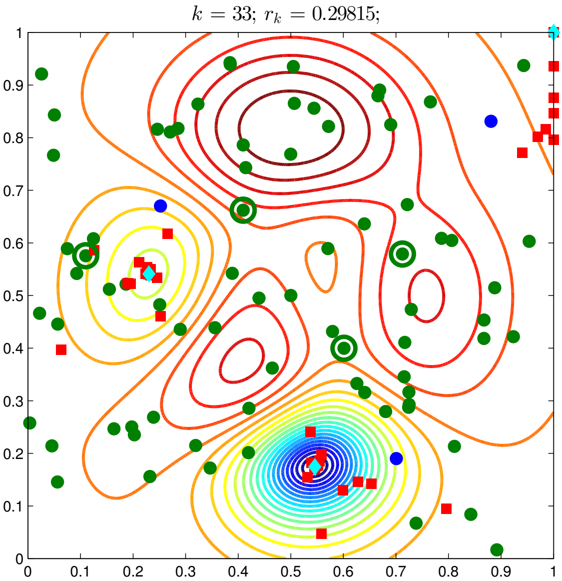


$k = 31;\ r_k = 0.3108;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Our Method

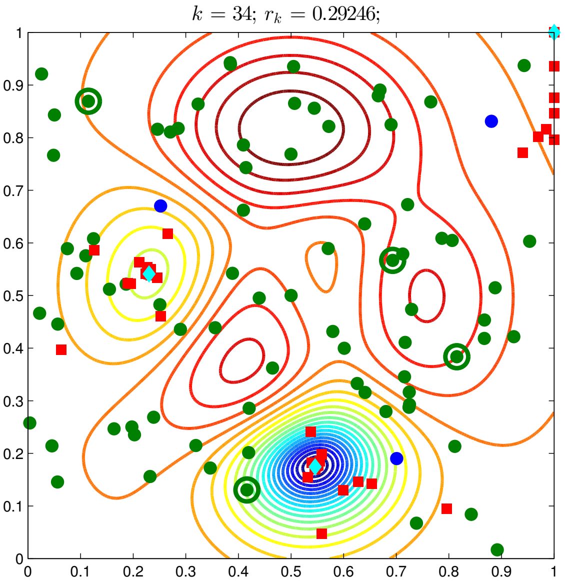


Our Method

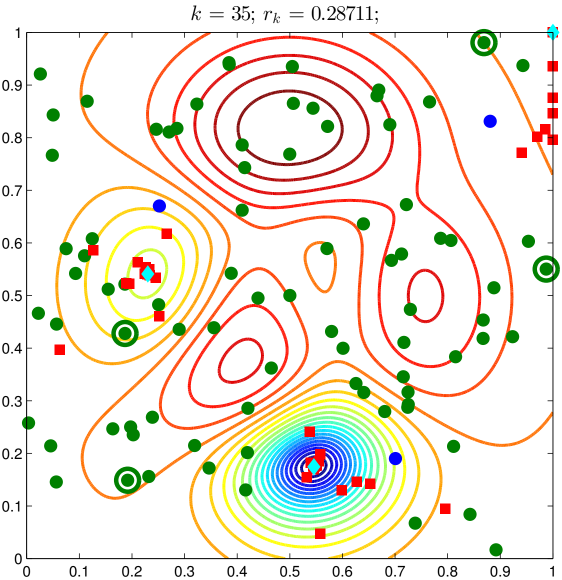


$k = 33$; $r_k = 0.29815$;
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Our Method

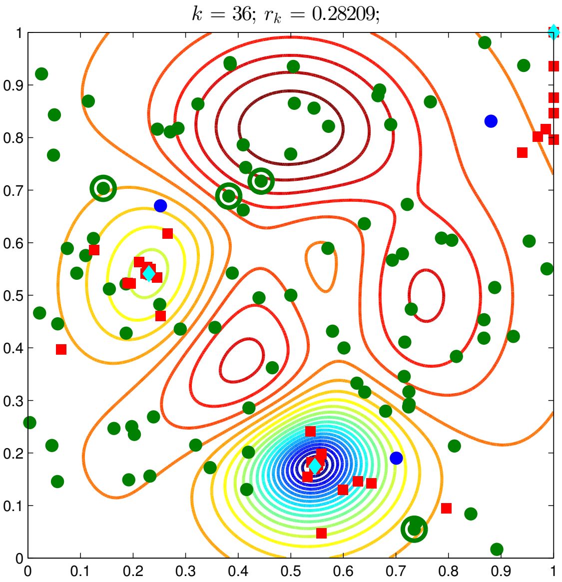


Our Method

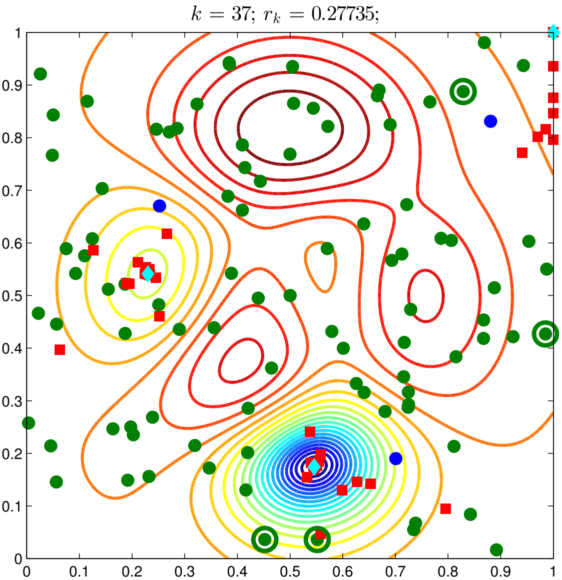


$k = 35; r_k = 0.28711;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

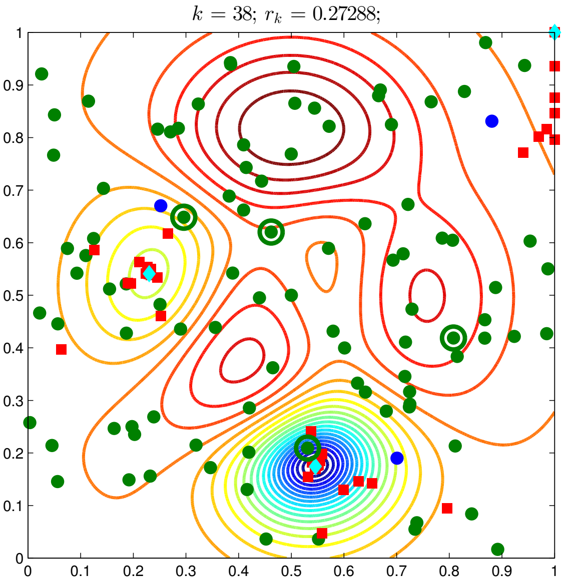
Our Method



Our Method



Our Method



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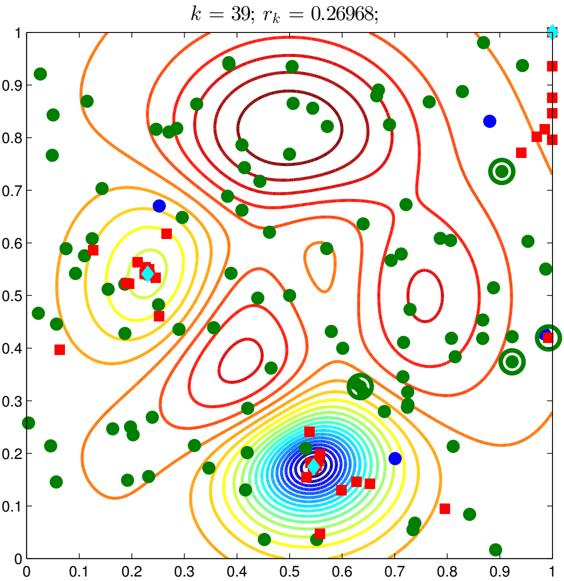
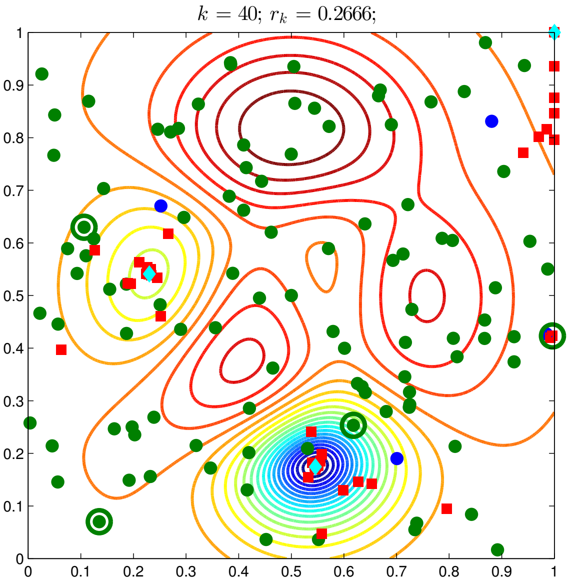
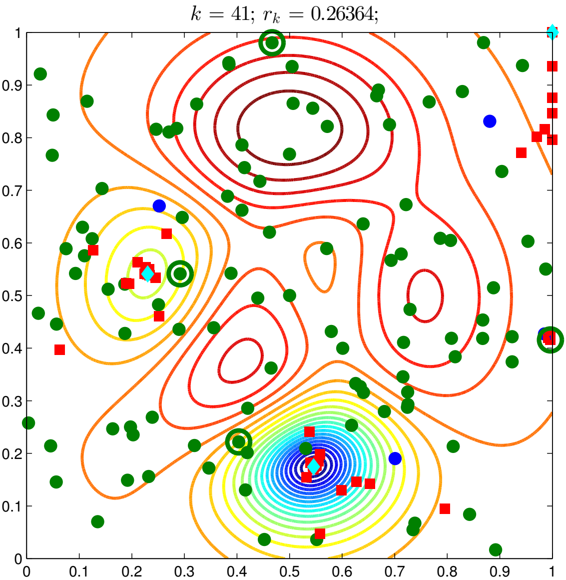


$k = 39;\ r_k = 0.26968;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

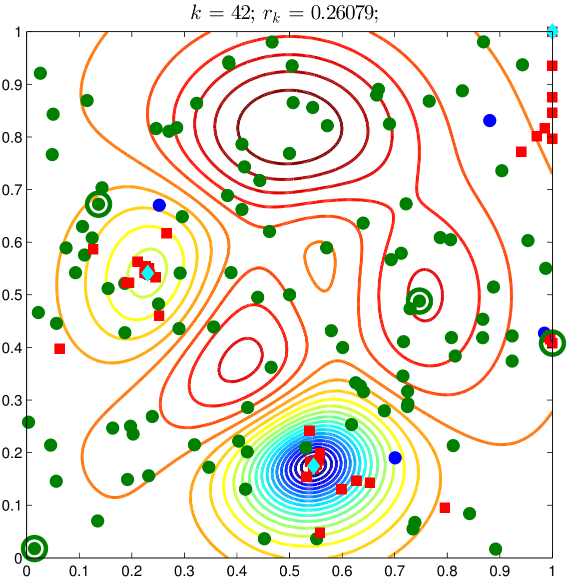
Our Method



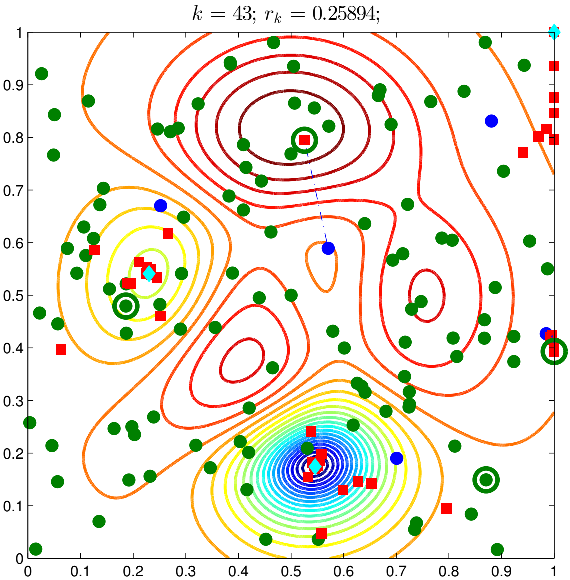
Our Method



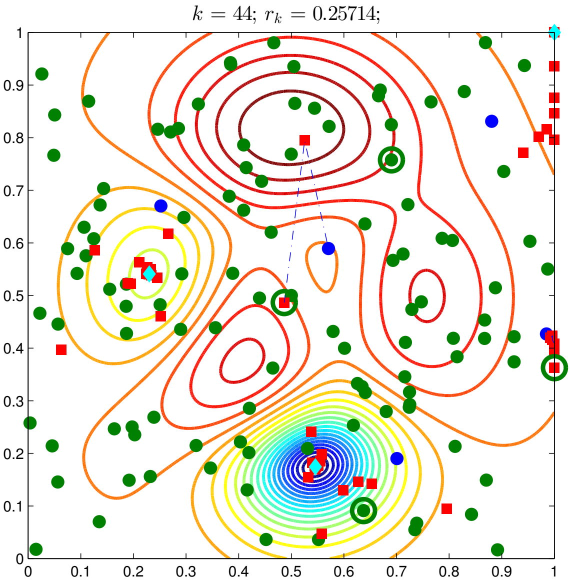
Our Method



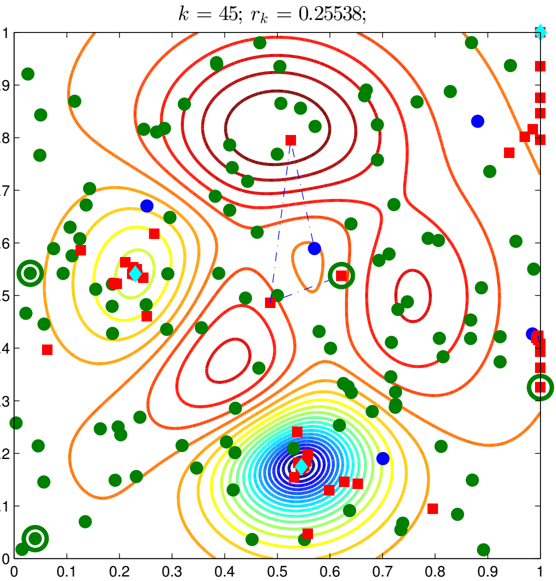
Our Method



Our Method



Our Method



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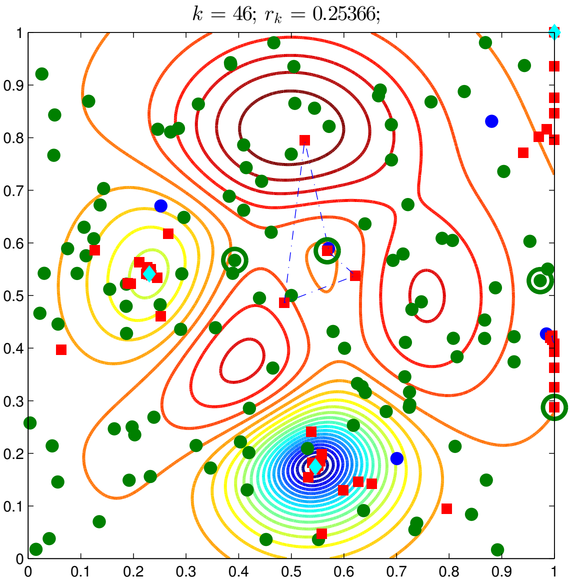
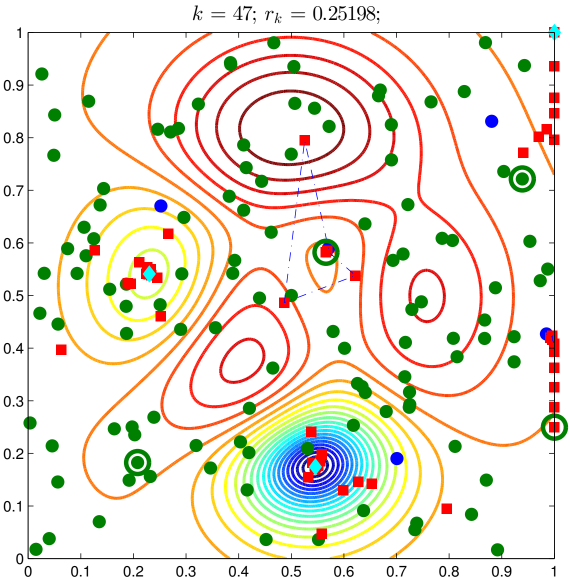
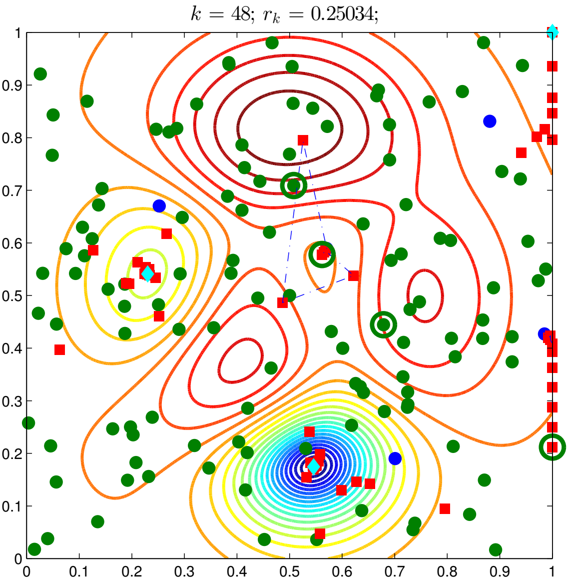


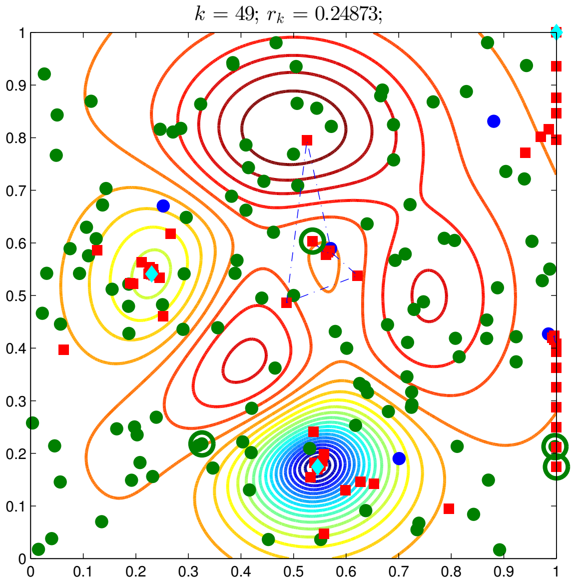
Our Method



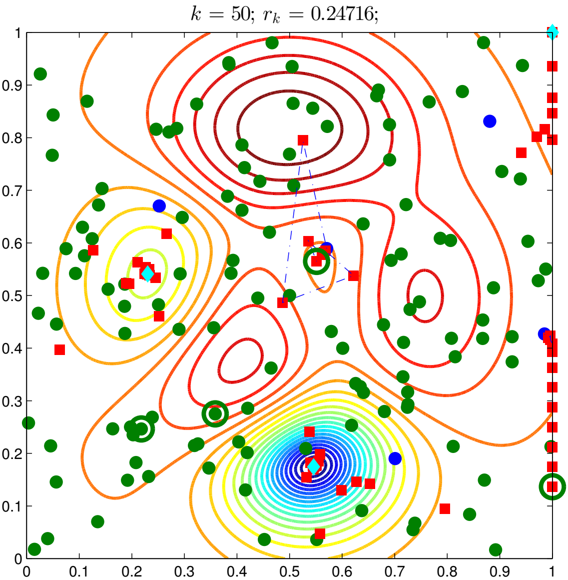
Our Method



Our Method

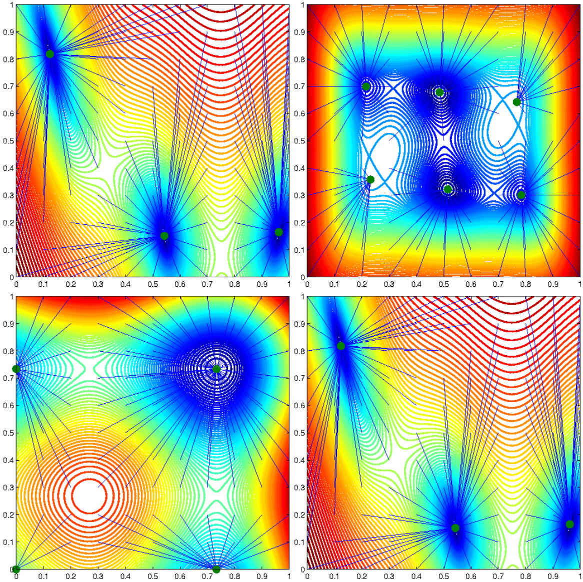


Our Method



$k = 50;\ r_k = 0.24716;$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Measuring Performance



ORBIT started from points in a 10x10 grid

Measuring Performance

Algorithms compared

- Ours (4 parallel workers)
- Direct (serial)
- pVTDirect (4 parallel workers)

- Since Ours involves a random sampling stream, each problem was duplicated 10 times.
- Each method evaluates the centroid first.

Measuring Performance

How would you measure how "efficiently" an algorithm finds multiple local minima?

Measuring Performance

Define

Let $\mathcal{X}^*$ be the set of all local minima of f.
Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*)|x^* \in \mathcal{X}^*\}$.
Let $x^*_{(i)}$ be the element of $\mathcal{X}^*$ corresponding to the value $f^*_{(i)}$.

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Measuring Performance

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Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*) | x^* \in \mathcal{X}^*\}$.
Let $x^*_{(i)}$ be the element of $\mathcal{X}^*$ corresponding to the value $f^*_{(i)}$.

A method has found the global minimum within a level $\tau > 0$ at batch iteration k if it has found a point $\hat{x}$ satisfying:

$$f(\hat{x}) - f^*_{(1)} \leq (1 - \tau) \left(f(x_0) - f^*_{(1)} \right),$$

where x_0 is the starting point for the problem.

Measuring Performance

Define

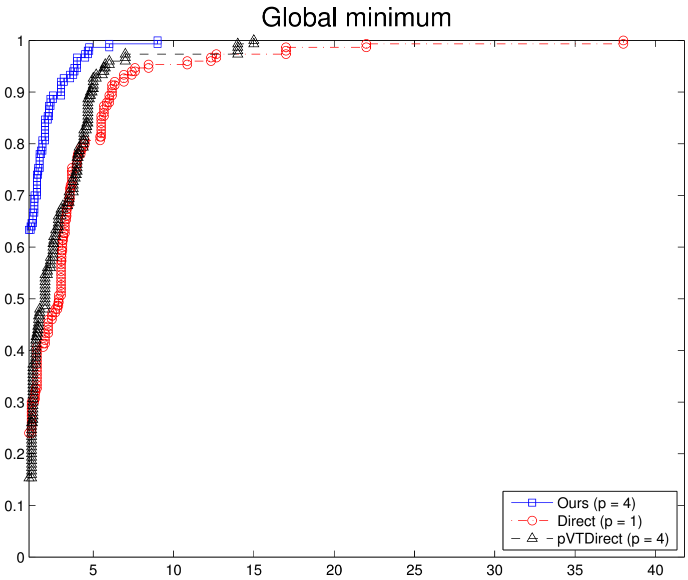
Let $\mathcal{X}^*$ be the set of all local minima of f.
Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*)|x^* \in \mathcal{X}^*\}$.
Let $x^*_{(i)}$ be the element of $\mathcal{X}^*$ corresponding to the value $f^*_{(i)}$.

A method has found the j best local minima within a level $\tau > 0$ at batch iteration k if:

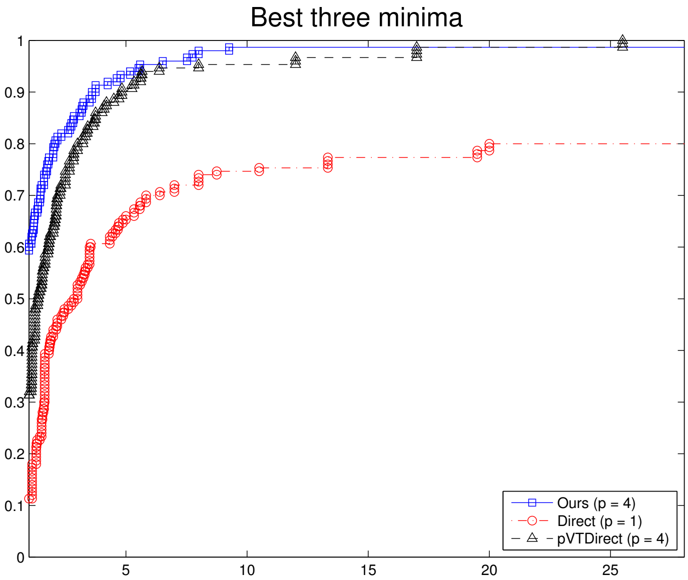
$$\left|\left\{x^*_{(1)}, \ldots, x^*_{(\bar{j})}\right\} \bigcap \left\{x^*_{(i)} | \exists \hat{x} \text{ s.t. } \left\|\hat{x} - x_{(i)}\right\| \leq \tau\right\}\right| \geq j$$

where $\bar{j}$ is the largest integer such that $f^*_{(\bar{j})} = f^*_{(j)}$.

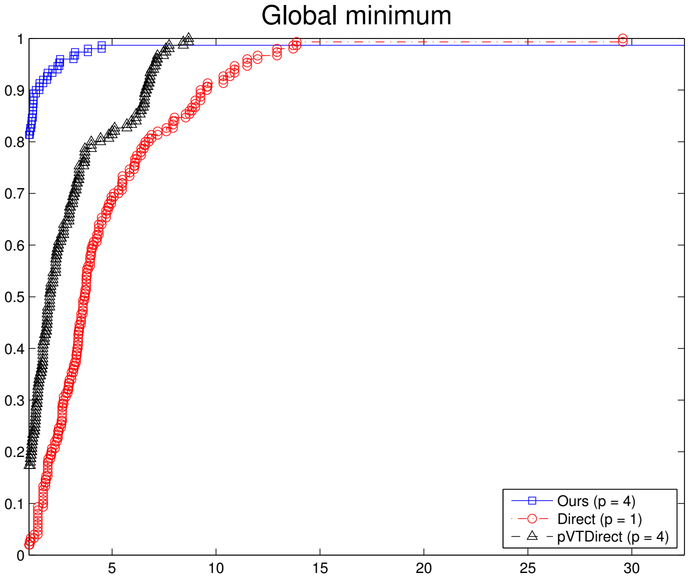
Measuring Performance: $\tau = 10^{-1}$



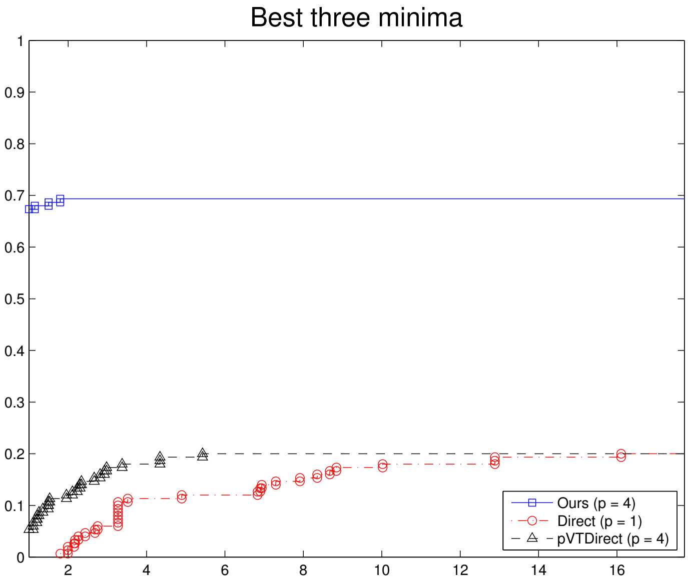
Measuring Performance: $\tau = 10^{-1}$



Measuring Performance: $\tau = 10^{-3}$



Measuring Performance: $\tau = 10^{-3}$



Conclusions and Future Work

Take Away:

- Derivative-free optimization is an active and applicable area of mathematics
- Local models efficiently use previous function evaluations
- Concurrent function evaluations can be used to help an algorithm find multiple local optima

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- Derivative-free optimization is an active and applicable area of mathematics
- Local models efficiently use previous function evaluations
- Concurrent function evaluations can be used to help an algorithm find multiple local optima

Working on:

- Industrial implementation of Our algorithm
- Accelerator design problems
- Developing rules for pausing local optimization runs

For students:

Computational math includes

- Applications
- Computer Programming
- Theory

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DFO is broad

- Geometry of evaluated points
- Analysis
- Stochastic/probabilistic functions
- Stochastic/probabilistic models
- Removing old points?

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Questions?

Other interests

- Sport Scheduling (Elitserien)
- Heavy-duty Vehicle Platooning
- Mathematics Outreach